

Supporting Information: Colorimetric Sensor Arrays for Volatile Organic Compounds

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ABSTRACT: The development of a low-cost, sensitive colorimetric sensor array for the detection and identification of volatile organic compounds (VOCs) is reported. Using an array composed of chemoresponsive dyes, enormous discriminatory power is possible in a simple device that can be imaged easily with an ordinary flat-bed scanner. Excellent differentiation of closely related organic compounds can be achieved, and a library of 100 VOCs is presented. The array discriminates among VOCs by probing a wide range of intermolecular interactions, including Lewis acid-base, Brønsted acid-base, metal ion coordination, hydrogen bonding, and dipolar interactions. Importantly, by proper choice of dyes and substrate, the array is essentially non-responsive to changes in humidity.

p. S2: **Table S1. Self-Query of Database**

p. S8: **Table S2. Complete Database of Array Responses to 100 Analytes.**

Table S1. Self-Query of Database

GOF = goodness of fit = 1 — (Unweighted Euclidean distance normalized by the maximum possible unweighted Euclidean distance).
The maximum possible unweighted Euclidean distance for 108 dimensions each with a range from -255 to +255 is
 $[108 * (511^2)]^{0.5} = 5310.47$

Database Entry	Closest Match	GOF
(d,l)-2-PPA 1	(d,l)-2-PPA AVG	0.991352
(d,l)-2-PPA 2	(d,l)-2-PPA AVG	0.994131
(d,l)-2-PPA 3	(d,l)-2-PPA AVG	0.993711
(d,l)-2-PPA AVG	(d,l)-2-PPA 2	0.994131
1,5-dimethylhexylamine 1	1,5-dimethylhexylamine Avg	0.987129
1,5-dimethylhexylamine 2	1,5-dimethylhexylamine Avg	0.990324
1,5-dimethylhexylamine 3	1,5-dimethylhexylamine Avg	0.992335
1,5-dimethylhexylamine Avg	1,5-dimethylhexylamine 3	0.992335
1-decanol 1	1-decanol AVG	0.997426
1-decanol 2	1-decanol AVG	0.997972
1-decanol 3	1-decanol AVG	0.997627
1-decanol AVG	1-decanol 2	0.997972
1-Hexylthiol 1	Avg 1-Hexylthiol	0.993507
1-Hexylthiol 2	Avg 1-Hexylthiol	0.993507
1-Hexylthiol avg	1-Hexylthiol 1	0.993507
1-Myrtenal 1	1-Myrtenal AVG	0.990239
1-Myrtenal 2	1-Myrtenal AVG	0.987873
1-Myrtenal 3	1-Myrtenal AVG	0.991093
1-Myrtenal AVG	1-Myrtenal 3	0.991093
1-octanethiol 1	Avg 1-octanethiol	0.996265
1-octanethiol 2	Avg 1-octanethiol	0.995561
1-octanethiol 3	Avg 1-octanethiol	0.996886
1-octanethiol avg	1-octanethiol 3	0.996886
1-octene 1	Avg 1-octene	0.997536
1-octene 2	Avg 1-octene	0.9972
1-octene 3	Avg 1-octene	0.997865
1-octene avg	1-octene 3	0.997865
1-Pentylthiol 1	Avg 1-Pentylthiol	0.995134
1-Pentylthiol 2	Avg 1-Pentylthiol	0.996234
1-Pentylthiol 3	Avg 1-Pentylthiol	0.993349
1-Pentylthiol avg	1-Pentylthiol 2	0.996234
2Clpropionicacid_1	2Clpropionicacid_Avg	0.994156
2Clpropionicacid_2	2Clpropionicacid_Avg	0.995455
2Clpropionicacid_3	2Clpropionicacid_Avg	0.993355
2Clpropionicacid_Avg	2Clpropionicacid_2	0.995455
2-decanol 1	2-decanol AVG	0.996103
2-decanol 2	2-decanol 3	0.995224
2-decanol 3	2-decanol AVG	0.996861
2-decanol AVG	2-decanol 3	0.996861
2-ethyl-1-hexylamine 1	Avg 2-ethyl-1-hexylamine	0.993846
2-ethyl-1-hexylamine 2	Avg 2-ethyl-1-hexylamine	0.994106
2-ethyl-1-hexylamine 3	Avg 2-ethyl-1-hexylamine	0.993611
2-ethyl-1-hexylamine avg	2-ethyl-1-hexylamine 2	0.994106
2-heptylamine 1	Avg 2-heptylamine	0.993858
2-heptylamine 2	Avg 2-heptylamine	0.995523
2-heptylamine 3	Avg 2-heptylamine	0.991555
2-heptylamine avg	2-heptylamine 2	0.995523
2-hexanol 1	2-hexanol AVG	0.99596
2-hexanol 2	2-hexanol AVG	0.996065
2-hexanol 3	2-hexanol AVG	0.99669
2-hexanol AVG	2-hexanol 3	0.99669
2-octanol 1	2-octanol AVG	0.993843
2-octanol 2	2-octanol AVG	0.995908
2-octanol 3	2-octanol AVG	0.996515
2-octanol AVG	2-octanol 3	0.996515
2-octanone 1	2-octanone 2	0.988849
2-octanone 2	Avg 2-octanone	0.99362
2-octanone 3	Avg 2-octanone	0.987802
2-octanone avg	2-octanone 2	0.99362
2-phenyl-1-propanol 1	2-phenyl-1-propanol AVG	0.996907
2-phenyl-1-propanol 2	2-phenyl-1-propanol AVG	0.997101
2-phenyl-1-propanol 3	2-phenyl-1-propanol AVG	0.997024
2-phenyl-1-propanol AVG	2-phenyl-1-propanol 2	0.997101
2-picoline 1	Avg 2-picoline	0.992127

2-picoline 2	Avg 2-picoline	0.996298
2-picoline 3	Avg 2-picoline	0.99286
2-picoline avg	2-picoline 2	0.996298
3,3-dimethyl-2-butanol 1	3,3-dimethyl-2-butanol AVG	0.996306
3,3-dimethyl-2-butanol 2	3,3-dimethyl-2-butanol AVG	0.995734
3,3-dimethyl-2-butanol 3	3,3-dimethyl-2-butanol AVG	0.995324
3,3-dimethyl-2-butanol AVG	3,3-dimethyl-2-butanol 1	0.996306
3,4-Lutidine 1	Avg 3,4-Lutidine	0.990037
3,4-Lutidine 3	Avg 3,4-Lutidine	0.990037
3,4-Lutidine avg	3,4-Lutidine 1	0.990037
3,5-dimethylaniline 1	Avg 3,5-dimethylaniline	0.991512
3,5-dimethylaniline 2	Avg 3,5-dimethylaniline	0.994312
3,5-dimethylaniline 3	Avg 3,5-dimethylaniline	0.993497
3,5-dimethylaniline avg	3,5-dimethylaniline 2	0.994312
3,5-Lutidine 1	Avg 3,5-Lutidine	0.98809
3,5-Lutidine 3	Avg 3,5-Lutidine	0.98809
3,5-Lutidine avg	3,5-Lutidine 1	0.98809
3-decanol 1	3-decanol AVG	0.996409
3-decanol 2	3-decanol AVG	0.997339
3-decanol 3	3-decanol AVG	0.996154
3-decanol AVG	3-decanol 2	0.997339
3-decanone 1	Avg 3-decanone	0.991624
3-decanone 2	Avg 3-decanone	0.993078
3-decanone 3	Avg 3-decanone	0.993915
3-decanone avg	3-decanone 3	0.993915
3-heptanone 1	Avg 3-heptanone	0.993883
3-heptanone 3	Avg 3-heptanone	0.993883
3-heptanone avg	3-heptanone 1	0.993883
3-hexanol 1	3-hexanol AVG	0.996221
3-hexanol 2	3-hexanol AVG	0.995652
3-hexanol 3	3-hexanol AVG	0.995957
3-hexanol AVG	3-hexanol 1	0.996221
3-picoline 1	Avg 3-picoline	0.994678
3-picoline 2	Avg 3-picoline	0.995699
3-picoline avg	3-picoline 2	0.995699
3-picoline3	Avg 3-picoline	0.995077
4-decanol 1	4-decanol AVG	0.996131
4-decanol 2	4-decanol AVG	0.995387
4-decanol 3	4-decanol AVG	0.996529
4-decanol AVG	4-decanol 3	0.996529
4-picoline 1	Avg 4-picoline	0.99399
4-picoline 2	Avg 4-picoline	0.994656
4-picoline 3	Avg 4-picoline	0.991998
4-picoline avg	4-picoline 2	0.994656
aceticacid_1	aceticacid_Avg	0.99428
aceticacid_2	aceticacid_Avg	0.993682
aceticacid_3	aceticacid_Avg	0.995076
aceticacid_Avg	aceticacid_3	0.995076
amylamine 1	Avg amylamine	0.992569
amylamine 2	Avg amylamine	0.99341
amylamine 3	Avg amylamine	0.992287
amylamine avg	amylamine 2	0.99341
aniline 1	aniline avg	0.994067
aniline 2	aniline avg	0.993882
aniline 3	aniline avg	0.995011
aniline avg	aniline 3	0.995011
Benzaldehyde 1	Benzaldehyde AVG	0.990255
Benzaldehyde 2	Benzaldehyde AVG	0.993041
Benzaldehyde 3	Benzaldehyde AVG	0.991656
Benzaldehyde AVG	Benzaldehyde 2	0.993041
benzene_1	benzene_3	0.995244
benzene_2	benzene_3	0.991711
benzene_3	benzene_1	0.995244
benzyl alcohol 1	benzyl alcohol AVG	0.997199
benzyl alcohol 2	benzyl alcohol AVG	0.997132
benzyl alcohol 3	benzyl alcohol AVG	0.997414
benzyl alcohol AVG	benzyl alcohol 3	0.997414
benzyl mercaptan 1	Avg benzyl mercaptan	0.997137
benzyl mercaptan 2	Avg benzyl mercaptan	0.996979
benzyl mercaptan 3	Avg benzyl mercaptan	0.995331
benzyl mercaptan avg	benzyl mercaptan 1	0.997137
benzylamine 1	Avg benzylamine	0.994329
benzylamine 2	Avg benzylamine	0.994329

benzylamine avg	benzylamine 1	0.994329
BrCH2CH2CO2H_1	BrCH2CH2CO2H_Avg	0.991435
BrCH2CH2CO2H_2	BrCH2CH2CO2H_Avg	0.995246
BrCH2CH2CO2H_3	BrCH2CH2CO2H_Avg	0.994398
BrCH2CH2CO2H_Avg	BrCH2CH2CO2H_2	0.995246
BrCH2CO2H_1	BrCH2CO2H_Avg	0.989206
BrCH2CO2H_2	BrCH2CO2H_3	0.994287
BrCH2CO2H_3	BrCH2CO2H_2	0.994287
BrCH2CO2H_Avg	BrCH2CO2H_2	0.993924
butanol_1	butanol_AVG	0.993904
butanol_2	butanol_AVG	0.995356
butanol_3	butanol_AVG	0.995753
butanol_AVG	butanol_3	0.995753
CF3CO2H_1	CF3CO2H_Avg	0.994412
CF3CO2H_2	CF3CO2H_Avg	0.994207
CF3CO2H_3	CF3CO2H_Avg	0.993215
CF3CO2H_Avg	CF3CO2H_1	0.994412
Cl3CCO2H_1	Cl3CCO2H_Avg	0.992815
Cl3CCO2H_2	Cl3CCO2H_Avg	0.993243
Cl3CCO2H_3	Cl3CCO2H_Avg	0.991873
Cl3CCO2H_Avg	Cl3CCO2H_2	0.993243
CICH2CO2H_1	CICH2CO2H_Avg	0.993935
CICH2CO2H_2	CICH2CO2H_Avg	0.995169
CICH2CO2H_3	CICH2CO2H_Avg	0.993731
CICH2CO2H_Avg	CICH2CO2H_2	0.995169
cycloheptanol_1	cycloheptanol_AVG	0.996491
cycloheptanol_2	cycloheptanol_AVG	0.997414
cycloheptanol_3	cycloheptanol_AVG	0.996352
cycloheptanol_AVG	cycloheptanol_2	0.997414
cyclohexanol_1	cyclohexanol_AVG	0.994915
cyclohexanol_2	cyclohexanol_AVG	0.995152
cyclohexanol_2	cyclohexanol_AVG	0.99418
cyclohexanol_3	cyclohexanol_AVG	0.995751
cyclohexanol_3	cyclohexanol_AVG	0.993997
cyclohexanol_AVG	cyclohexanol_1	0.996288
cyclohexanol_AVG	cyclohexanol_1	0.994915
cyclohexanol_1	cyclohexanol_AVG	0.996288
cyclohexene_1	Avg cyclohexene	0.996228
cyclohexene_2'	Avg cyclohexene	0.995906
cyclohexene_3	Avg cyclohexene	0.995718
cyclohexene_avg	cyclohexene_1	0.996228
cyclohexylthiol_1	Avg cyclohexylthiol	0.996336
cyclohexylthiol_2	Avg cyclohexylthiol	0.995513
cyclohexylthiol_3	Avg cyclohexylthiol	0.997384
cyclohexylthiol_avg	cyclohexylthiol_3	0.997384
cyclooctylamine_1	Avg cyclooctylamine	0.991691
cyclooctylamine_2	Avg cyclooctylamine	0.992459
cyclooctylamine_3	Avg cyclooctylamine	0.990951
cyclooctylamine_avg	cyclooctylamine_2	0.992459
cyclopentanol_1	cyclopentanol_AVG	0.994498
cyclopentanol_2	cyclopentanol_AVG	0.99572
cyclopentanol_3	cyclopentanol_AVG	0.99575
cyclopentanol_AVG	cyclopentanol_3	0.99575
Decylaldehyde_1	Decylaldehyde_AVG	0.995068
Decylaldehyde_2	Decylaldehyde_AVG	0.990976
Decylaldehyde_3	Decylaldehyde_AVG	0.995106
Decylaldehyde_4	Decylaldehyde_AVG	0.99237
Decylaldehyde_AVG	Decylaldehyde_3	0.995106
decylamine_1	Avg decylamine	0.993499
decylamine_2	Avg decylamine	0.990463
decylamine_3	Avg decylamine	0.994872
decylamine_avg	decylamine_3	0.994872
dibenzylamine_1	dibenzylamine.avg	0.99586
dibenzylamine_2	dibenzylamine_1	0.994763
dibenzylamine_3	dibenzylamine.avg	0.99171
dibenzylamine.avg	dibenzylamine_1	0.99586
dicyclohexylamine_1	dicyclohexylamine.avg	0.99284
dicyclohexylamine_2	dicyclohexylamine.avg	0.995687
dicyclohexylamine_3	dicyclohexylamine.avg	0.994967
dicyclohexylamine.avg	dicyclohexylamine_2	0.995687
diisobutylamine_1	diisobutylamine_avg	0.99326
diisobutylamine_3	diisobutylamine_avg	0.99326
diisobutylamine_avg	diisobutylamine_1	0.99326

dimethylphenylphosphine 1	dimethylphenylphosphine AVG	0.995968
dimethylphenylphosphine 3	dimethylphenylphosphine AVG	0.995977
dimethylphenylphosphine 2	dimethylphenylphosphine AVG	0.996161
dimethylphenylphosphine AVG	dimethylphenylphosphine 2	0.996161
di-n-butylamine 1	di-n-butylamine avg	0.993988
di-n-butylamine 2	di-n-butylamine avg	0.994683
di-n-butylamine 3	di-n-butylamine avg	0.993095
di-n-butylamine avg	di-n-butylamine 2	0.994683
dipropylamine 1	Avg dipropylamine	0.992281
dipropylamine 2	Avg dipropylamine	0.993847
dipropylamine 3	Avg dipropylamine	0.994082
dipropylamine avg	dipropylamine 3	0.994082
disecbutylamine 1	disecbutylamine avg	0.995171
disecbutylamine 2	disecbutylamine avg	0.994153
disecbutylamine 3	disecbutylamine avg	0.993385
disecbutylamine avg	disecbutylamine 1	0.995171
dodecane 1	Avg dodecane	0.996764
dodecane 2	Avg dodecane	0.997322
dodecane 3	Avg dodecane	0.997335
dodecane avg	dodecane 3	0.997335
dodecanol 1	dodecanol 3	0.99645
dodecanol 2	dodecanol 3	0.996138
dodecanol 3	dodecanol 1	0.99645
dodecanol AVG	dodecanol 1	0.995756
ethanol 1	ethanol AVG	0.993599
ethanol 2	ethanol AVG	0.993524
ethanol 3	ethanol AVG	0.995061
ethanol AVG	ethanol 3	0.995061
Ethyl benzoate 1	Ethyl benzoate AVG	0.994788
Ethyl benzoate 2	Ethyl benzoate AVG	0.994652
Ethyl benzoate 3	Ethyl benzoate AVG	0.993852
Ethyl benzoate AVG	Ethyl benzoate 1	0.994788
Ethyl nonanoate 1	Ethyl nonanoate AVG	0.995198
Ethyl nonanoate 2	Ethyl nonanoate AVG	0.996218
Ethyl nonanoate 3	Ethyl nonanoate AVG	0.994168
Ethyl nonanoate AVG	Ethyl nonanoate 2	0.996218
formicacid_1	formicacid_Avg	0.995392
formicacid_2	formicacid_Avg	0.994311
formicacid_3	formicacid_Avg	0.994749
formicacid_Avg	formicacid_1	0.995392
Heptaldehyde 1	Heptaldehyde AVG	0.99581
Heptaldehyde 2	Heptaldehyde AVG	0.99581
Heptaldehyde AVG	Heptaldehyde 1	0.99581
heptanoicacid_1	heptanoicacid_Avg	0.993951
heptanoicacid_2	heptanoicacid_Avg	0.993452
heptanoicacid_3	heptanoicacid_Avg	0.993101
heptanoicacid_Avg	heptanoicacid_1	0.993951
heptanol 1	heptanol AVG	0.996013
heptanol 2	heptanol AVG	0.99519
heptanol 3	heptanol AVG	0.994654
heptanol 4	heptanol AVG	0.994839
heptanol 5	heptanol AVG	0.994641
heptanol AVG	heptanol 1	0.996013
heptylamine 1	heptylamine avg	0.99517
heptylamine 2	heptylamine avg	0.995344
heptylamine 3	heptylamine avg	0.994205
heptylamine avg	heptylamine 2	0.995344
hexadecane 1	hexadecane avg	0.997963
hexadecane 2	hexadecane avg	0.99762
hexadecane 3	hexadecane avg	0.998299
hexadecane avg	hexadecane 3	0.998299
Hexanal 1	Hexanal AVG	0.993666
Hexanal 3	Hexanal AVG	0.995394
Hexanal 4	Hexanal AVG	0.994677
Hexanal AVG	Hexanal 3	0.995394
hexanoicacid_1	hexanoicacid_Avg	0.995004
hexanoicacid_2	hexanoicacid_Avg	0.995794
hexanoicacid_3	hexanoicacid_Avg	0.994883
hexanoicacid_Avg	hexanoicacid_2	0.995794
hexanol 1	hexanol AVG	0.995797
hexanol 3	hexanol AVG	0.995364
hexanol 5	hexanol 4	0.994773
hexanol AVG	hexanol 1	0.995797

hexanol_2	hexanol_AVG	0.99541
hexanol_4	hexanol_5	0.994773
Me2CHCO2H_1	Me2CHCO2H_Avg	0.995473
Me2CHCO2H_2	Me2CHCO2H_Avg	0.996525
Me2CHCO2H_3	Me2CHCO2H_Avg	0.995775
Me2CHCO2H_Avg	Me2CHCO2H_2	0.996525
Me3CCO2H_1	Me3CCO2H_Avg	0.994323
Me3CCO2H_2	Me3CCO2H_Avg	0.996007
Me3CCO2H_3	Me3CCO2H_Avg	0.994943
Me3CCO2H_Avg	Me3CCO2H_2	0.996007
Methyl benzoate_3	Methyl benzoate_AVG	0.995217
Methyl benzoate_4	Methyl benzoate_AVG	0.995217
Methyl benzoate_AVG	Methyl benzoate_4	0.995217
Methyl octanoate_1	Methyl octanoate_AVG	0.993581
Methyl octanoate_2	Methyl octanoate_AVG	0.995286
Methyl octanoate_3	Methyl octanoate_AVG	0.993389
Methyl octanoate_AVG	Methyl octanoate_2	0.995286
n,n-dimethylbenzylamine_1	Avg n,n-dimethylbenzylamine	0.993479
n,n-dimethylbenzylamine_2	Avg n,n-dimethylbenzylamine	0.995276
n,n-dimethylbenzylamine_3	Avg n,n-dimethylbenzylamine	0.994062
n,n-dimethylbenzylamine_avg	n,n-dimethylbenzylamine_2	0.995276
N,N-dimethylhexylamine_1	N,N-dimethylhexylamine_Avg	0.993581
N,N-dimethylhexylamine_2	N,N-dimethylhexylamine_Avg	0.994832
N,N-dimethylhexylamine_3	N,N-dimethylhexylamine_Avg	0.993241
N,N-dimethylhexylamine_Avg	N,N-dimethylhexylamine_2	0.994832
n-octylamine_1	Avg n-octylamine	0.993332
n-octylamine_2	Avg n-octylamine	0.992872
n-octylamine_3	Avg n-octylamine	0.991482
n-octylamine_avg	n-octylamine_1	0.993332
nonanol_2	nonanol_AVG	0.997323
nonanol_3	nonanol_AVG	0.996915
nonanol_AVG	nonanol_2	0.997323
nonanol_1	nonanol_AVG	0.995081
Nonylaldehyde_1	Nonylaldehyde_AVG	0.994271
Nonylaldehyde_2	Nonylaldehyde_AVG	0.995762
Nonylaldehyde_3	Nonylaldehyde_AVG	0.993808
Nonylaldehyde_AVG	Nonylaldehyde_2	0.995762
nonylamine_1	nonylamine_avg	0.994943
nonylamine_2	nonylamine_avg	0.994943
nonylamine_avg	nonylamine_1	0.994943
octane_1	Avg octane	0.996536
octane_2	Avg octane	0.996472
octane_3	Avg octane	0.997125
octane_avg	octane_3	0.997125
octanoicacid_1	octanoicacid_Avg	0.993489
octanoicacid_2	octanoicacid_Avg	0.997082
octanoicacid_3	octanoicacid_Avg	0.994745
octanoicacid_Avg	octanoicacid_2	0.997082
octanol_1	octanol_AVG	0.996793
octanol_2	octanol_AVG	0.997219
octanol_3	octanol_AVG	0.997009
octanol_AVG	octanol_2	0.997219
Octylaldehyde_2	Octylaldehyde_AVG	0.993187
Octylaldehyde_3	Octylaldehyde_AVG	0.992733
Octylaldehyde_4	Octylaldehyde_AVG	0.994263
Octylaldehyde_AVG	Octylaldehyde_4	0.994263
o-Tolualdehyde_1	o-Tolualdehyde_AVG	0.992581
o-Tolualdehyde_2	o-Tolualdehyde_AVG	0.992581
o-Tolualdehyde_AVG	o-Tolualdehyde_2	0.992581
paraxylene_1	paraxylene_Avg	0.995276
paraxylene_2	paraxylene_Avg	0.995449
paraxylene_3	paraxylene_Avg	0.995772
paraxylene_Avg	paraxylene_3	0.995772
pentanoicacid_1	pentanoicacid_Avg	0.990752
pentanoicacid_2	pentanoicacid_Avg	0.995663
pentanoicacid_3	pentanoicacid_Avg	0.991644
pentanoicacid_Avg	pentanoicacid_2	0.995663
pentanol_1	pentanol_AVG	0.996608
pentanol_2	pentanol_AVG	0.996645
pentanol_4	pentanol_AVG	0.996401
pentanol_AVG	pentanol_2	0.996645
perfluoroctanoicacid_1	perfluoroctanoicacid_Avg	0.994117
perfluoroctanoicacid_2	perfluoroctanoicacid_Avg	0.99238

perfluoroctanoicacid_3	perfluoroctanoicacid_Avg	0.993582
perfluoroctanoicacid_Avg	perfluoroctanoicacid_1	0.994117
phenol_1	phenol_AVG	0.995209
phenol_2	phenol_AVG	0.995947
phenol_3	phenol_AVG	0.995906
phenol_AVG	phenol_2	0.995947
propionicacid_1	propionicacid_Avg	0.990486
propionicacid_2	propionicacid_Avg	0.994793
propionicacid_3	propionicacid_Avg	0.994793
propionicacid_Avg	propionicacid_3	0.994793
pyridine_1	Avg pyridine	0.993302
pyridine_2	Avg pyridine	0.991882
pyridine_3	Avg pyridine	0.99296
pyridine_avg	pyridine_1	0.993302
tetradecane_1	Avg tetradecane	0.997703
tetradecane_2	Avg tetradecane	0.997918
tetradecane_3	Avg tetradecane	0.99801
tetradecane_avg	tetradecane_3	0.99801
t-octylamine_1	t-octylamine_avg	0.994121
t-octylamine_3	t-octylamine_avg	0.994121
t-octylamine_avg	t-octylamine_1	0.994121
toluene_1	toluene_Avg	0.99537
toluene_2	toluene_Avg	0.997391
toluene_3	toluene_Avg	0.995837
toluene_Avg	toluene_2	0.997391
trans-5-decene_2	trans-5-deceneAvg	0.993842
trans-5-decene_3	trans-5-deceneAvg	0.995004
trans-5-decene1	trans-5-deceneAvg	0.995756
trans-5-deceneAvg	trans-5-decene1	0.995756
triethylamine_1	triethylamine average	0.990451
triethylamine_2	triethylamine average	0.991775
triethylamine_3	triethylamine average	0.992029
triethylamine average	triethylamine_3	0.992029
tri-n-butylphosphine_1	tri-n-butylphosphine_AVG	0.993637
tri-n-butylphosphine_2	tri-n-butylphosphine_AVG	0.993392
tri-n-butylphosphine_3	tri-n-butylphosphine_AVG	0.99292
tri-n-butylphosphine_4	tri-n-butylphosphine_AVG	0.993891
tri-n-butylphosphine_AVG	tri-n-butylphosphine_4	0.993891
undecylamine_1	Avg undecylamine	0.993849
undecylamine_2	Avg undecylamine	0.995945
undecylamine_3	Avg undecylamine	0.992601
undecylamine_avg	undecylamine_2	0.995945

Table S2. Complete Database of Array Responses to 100 Analytes.

For each entry, the following 108 numbers represent the change in R, G, and B values of the 36 dye array (i.e., after exposure – before exposure), dye by dye from top left to bottom right of the array.

octanoicacid_1	0.1	0.7	0.5	-9.8	-0.3	3.6	-1.4	-1.4	0.9	-1.6	0.6	-1.5	0.2	1.2	2.3	-1.6	0.5	0.9	-0.7	-0.7	0.9			
	-1.8	-4.2	-5.9	-1.5	-1.8	-1.7	-1.8	-1.9	0.8	-1.0	0.6	-1.3	0.9	0.8	0.4	-0.6	6.6	11.2	-1.8	3.5	1.6	-0.6	1.9	16.3
	0.3	9.7	13.7	-1.0	3.5	-1.5	-0.3	3.9	5.6	0.0	2.4	11.3	0.8	10.3	7.6	0.8	-0.3	4.7	-0.4	-54.2	-14.6	88.8	91.1	-62.3
	29.7	39.5	-49.5	55.2	52.9	-23.2	8.4	74.1	5.7	36.2	93.0	-15.8	66.1	83.4	-14.2	0.3	28.2	113.4	1.5	-0.2	-1.4	25.2	33.2	13.3
	89.4	75.7	36.1	8.0	26.0	20.0	32.2	41.4	3.8	-1.6	4.8	2.4	1.7	3.9	9.2									
octanoicacid_2	0.3	0.9	2.2	-12.7	-0.7	5.5	1.5	0.8	5.0	1.9	1.0	2.8	0.3	0.5	-0.6	-1.6	-0.1	0.6	-0.7	1.1	2.8			
	1.0	0.4	-0.2	2.5	3.1	3.9	2.0	-2.0	2.4	-1.6	1.7	-1.3	0.2	1.1	1.7	0.2	7.1	11.4	0.6	2.5	2.6	-0.2	1.6	23.2
	2.5	8.6	13.9	0.5	3.6	0.0	-0.4	5.2	11.4	-0.7	2.5	13.0	0.4	7.5	7.9	-0.9	-1.3	4.0	-0.4	-51.2	-13.6	85.1	88.3	-64.5
	27.9	37.7	-54.9	34.9	31.2	-19.1	9.7	67.0	2.1	36.3	92.0	-18.5	68.0	80.0	-14.5	-2.8	28.8	107.2	1.0	-1.1	0.5	23.5	31.2	14.2
	105.2	84.3	42.8	5.7	16.8	15.0	39.1	46.7	-0.5	-2.2	3.2	2.9	0.4	1.9	5.8									
octanoicacid_3	-0.6	-0.4	-0.1	-7.1	3.0	8.9	0.8	-1.2	4.6	0.5	1.1	3.4	1.7	0.4	2.2	-3.8	-0.3	1.0	-0.6	-0.8	5.0			
	-0.1	0.1	3.2	1.4	1.2	2.1	3.5	3.2	5.1	-0.4	1.6	2.1	0.0	1.3	4.0	1.3	6.1	8.5	1.7	3.2	6.5	1.0	4.2	21.1
	0.6	7.2	13.4	-0.3	4.7	2.0	-0.8	7.0	9.5	1.3	2.4	12.4	0.0	7.2	5.1	0.8	0.7	4.4	-1.0	-46.8	-10.0	79.8	82.6	-59.8
	28.1	38.1	-46.1	29.8	26.8	-16.9	8.5	63.3	0.6	32.5	84.3	-20.9	62.5	74.8	-15.3	-1.2	25.6	104.3	0.9	0.6	0.7	25.7	34.0	12.2
	112.4	88.6	45.8	4.1	17.1	14.4	40.5	52.0	0.7	-2.6	3.6	-0.4	-0.3	5.8	9.2									
octanoicacid_Avg	0.0	0.4	0.9	-9.9	0.7	6.0	0.3	-0.6	3.5	0.3	0.9	1.6	0.8	0.7	1.3	-2.3	0.0	0.9	-0.6	-0.1	2.9			
	-0.3	-1.2	-1.0	0.8	0.9	1.4	1.2	-0.2	2.8	-1.0	1.3	-0.2	0.4	1.1	2.0	0.3	6.6	10.4	0.2	3.1	3.6	0.1	2.5	20.2
	1.1	8.5	13.7	-0.3	3.9	0.2	-0.5	5.4	8.8	0.2	2.4	12.2	0.4	8.3	6.9	0.2	-0.3	4.3	-0.6	-50.7	-12.8	84.6	87.3	-62.2
	28.6	38.4	-50.2	39.9	36.9	-19.8	8.9	68.1	2.8	35.0	89.8	-18.4	65.6	79.4	-14.6	-1.2	27.5	108.3	1.1	-0.2	-0.1	24.8	32.8	13.2
	102.3	82.9	41.6	5.9	20.0	16.4	37.3	46.7	1.4	-2.1	3.9	1.6	0.6	3.9	8.1									
heptanoicacid_1	6.0	5.4	6.3	3.1	1.5	3.6	2.4	1.4	5.7	2.5	0.6	5.6	0.6	-0.2	1.2	-2.3	-0.4	3.1	0.3	1.9	1.3			
	1.8	-2.9	-6.3	-0.4	-1.4	1.3	-0.4	-0.5	2.0	-0.1	1.2	1.0	1.5	0.7	1.6	1.1	10.5	8.6	1.4	3.8	4.0	-1.0	1.3	25.7
	1.1	12.9	31.1	0.1	5.9	0.9	1.1	3.3	7.5	4.1	3.1	13.2	-0.1	10.8	10.6	0.6	-1.1	5.4	-0.3	-76.2	-16.0	103.9	108.9	-70.0
	41.8	49.7	-59.8	71.1	75.6	-15.7	11.0	80.1	6.5	41.1	96.9	-21.6	75.2	89.9	-19.6	-0.3	31.9	116.1	3.3	-3.3	-1.5	26.8	35.0	10.2
	114.3	90.2	47.9	7.2	32.4	32.3	38.6	45.5	-3.3	-9.5	2.6	-1.3	0.6	0.8	1.7									
heptanoicacid_2	0.1	1.7	1.2	0.8	1.1	1.3	0.0	-0.1	4.6	-0.4	-2.2	2.2	0.6	0.7	0.8	-5.8	-0.6	2.0	-0.4	1.7	-1.9			
	1.7	-0.3	-1.0	0.2	-0.6	4.1	-0.5	-1.9	-0.1	0.9	2.4	2.4	0.8	1.8	2.1	-0.4	4.6	7.2	-1.2	4.2	2.4	-3.0	0.6	26.4
	-1.5	9.3	40.4	0.1	4.2	1.4	-1.4	4.3	20.3	3.0	2.1	5.3	-0.5	7.3	8.7	-2.9	-3.4	6.1	-3.1	-70.0	-14.6	98.6	106.0	-66.1
	57.2	59.3	-60.7	57.4	57.1	-23.7	8.8	70.0	3.7	35.9	85.0	-21.5	63.1	70.8	-16.5	-4.8	28.3	112.2	-0.6	-5.4	-2.7	19.2	26.4	7.1
	100.1	84.4	40.7	6.6	29.9	25.7	35.0	40.6	1.6	-10.1	1.0	-1.1	-2.3	-2.4	-4.1									
heptanoicacid_3	-3.3	-0.5	-2.5	-8.9	-1.9	1.9	-8.6	-4.7	-3.8	-9.5	-5.6	-5.9	-5.3	-2.4	-0.5	-8.5	-2.9	0.9	-0.9	0.1	1.9			
	-1.6	-4.0	-3.6	-2.9	-4.3	0.5	-0.3	-3.1	2.1	-3.0	-0.7	-1.8	-3.2	-1.1	1.2	-0.8	6.3	5.3	-1.0	3.9	2.3	-3.6	-1.1	22.7
	-2.8	8.1	20.3	-0.8	7.7	3.9	-3.1	5.8	18.2	-1.0	0.9	14.2	0.9	6.7	10.0	-0.8	-4.1	8.9	1.1	-70.1	-12.7	103.0	113.2	-67.3
	59.2	62.1	-57.4	63.4	64.6	-16.6	11.9	77.8	6.1	39.4	90.9	-19.5	73.3	89.8	-16.8	-0.1	30.4	127.0	2.8	-1.8	-7.8	24.2	31.4	10.1
	109.9	81.9	50.8	6.7	38.7	39.8	36.5	71.0	8.0	-4.9	6.3	-0.1	2.2	1.8	3.3									
heptanoicacid_Avg	1.0	2.2	1.7	-1.7	0.2	2.3	-2.1	-1.1	2.2	-2.5	-2.4	0.6	-1.4	-0.6	0.5	-5.6	-1.3	2.0	-0.4	1.3				
	0.4	0.6	-2.4	-3.6	-1.0	-2.1	2.0	-0.4	-1.9	1.3	-0.7	0.9	0.5	-0.3	0.5	1.6	0.0	7.2	7.1	-0.3	4.0	2.9	-2.5	0.3
	24.9	-1.1	10.1	30.6	-0.2	5.9	2.1	-1.1	4.5	15.3	2.1	2.0	10.9	0.1	8.3	9.8	-1.0	-2.8	6.8	-0.8	-72.1	-14.4	101.9	109.4
	-67.8	52.8	57.0	-59.3	64.0	65.8	-18.7	10.6	76.0	5.5	38.8	90.9	-20.9	70.5	83.5	-17.6	-1.8	30.2	118.4	1.9	-3.5	-4.0	23.4	31.0
	9.1	108.1	85.5	46.5	6.8	33.7	32.6	36.7	52.4	2.1	-8.2	3.3	-0.8	0.2	0.1	0.3								
BrCH2CH2CO2H_1	-7.2	-5.1	-4.9	-10.5	-1.7	1.5	-3.5	-3.1	-1.0	-4.0	-1.6	-1.8	0.1	-0.2	2.2	-2.5	-1.1	2.0	-1.1	-1.6				
	0.5	-1.3	-4.9	-6.5	-2.0	-1.4	-1.6	0.7	-1.5	0.0	-2.9	0.6	-1.6	-2.1	-1.3	0.1	-1.3	-0.9	-0.3	-0.1	1.2	0.5	-1.9	-1.8
	2.4	-2.0	0.1	0.8	-2.0	0.8	1.9	-3.0	-3.8	-9.4	4.6	4.2	4.7	1.5	1.9	1.7	-0.2	-4.9	3.8	1.1	-74.5	-21.4	96.6	103.8
	-64.6	48.6	56.0	-61.1	46.3	44.9	-18.9	12.3	76.6	3.9	40.0	93.3	-20.2	71.0	86.4	-21.0	-3.6	31.8	113.5	-0.7	-9.4	0.3	23.7	31.0
	12.3	116.5	85.8	57.6	7.3	42.4	50.5	42.4	95.6	48.2	-8.6	7.3	1.5	1.6	4.6									
BrCH2CH2CO2H_2	1.2	0.4	1.4	-5.2	1.0	3.1	-1.3	0.2	2.7	0.1	0.9	2.0	0.9	0.2	1.7	-1.9	0.6	1.9	0.9	-3.3	0.2	-4.3	-5.6	-3.7
	4.8	-3.4	-0.6	5.1	-0.6	0.8	-2.8	-3.3	-1.6	-0.9	0.8	0.9	4.0	-1.0	1.6	0.8	-2.7	-5.6	3.1	-1.7	-69.1	-22.4	86.5	91.3
	-61.6	38.2	46.0	-56.2	18.4	17.4	-10.0	7.6	63.5	1.0	34.8	81.5	-20.3	63.5	77.9	-20.2	0.3	22.7	111.2	-0.9	-8.4	-3.4	20.5	28.9
	8.9	111.9	82.3	48.5	4.6	28.5	30.1	39.0	84.8	33.2	-12.0	1.2	-0.8	-1.3	-0.3	0.2								
BrCH2CH2CO2H_3	-1.1	1.1	0.2	-6.3	0.0	8.8	0.2	0.5	3.1	-1.2	1.2	2.7	0.8	0.6	0.9	-1.1	1.3	5.0	0.9	1.3				
	1.3	0.1	-0.7	-3.5	1.0	0.9	2.3	2.5	0.6	2.6	0.2	1.8	1.5	0.8	1.7	2.2	-0.9	-1.8	-3.4	-0.3	0.3	-1.7	-0.4	-1.3
	2.5	-1.2	-1.0	1.4	-0.6	0.8	4.3	-1.0	-1.0	-5.4	-2.4	-1.9	2.5	-1.2	-1.6	-0.1	-9.5	-6.2	0.9	-0.9	-71.9	-18.4	89.3	95.1
	-67.9	36.5	48.5	-57.3	18.5	17.9	-10.4	10.5	66.5	0.8	35.1	87.2	-21.0	68.4	79.4	-22.5	-1.7	27.5	102.1	0.8	-5.7	0.3	19.1	25.0
	4.4	111.8	82.5	50.3	2.0	23.1	23.3	40.1	80.7	24.8	-8.0	2.4	-1.5	-3.6	-1.0	-1.4								
BrCH2CH2CO2H_Avg	-2.4	-1.2	-1.1	-7.3	-0.2	4.5	-1.5	-0.8</td																

100.8	89.5	-60.5	71.1	75.0	-20.5	8.7	70.0	15.5	34.1	82.9	-17.4	58.9	68.8	-11.1	0.6	25.1	112.7	2.0	5.0	-5.5	20.1	28.6	13.9		
113.9	86.6	59.2	8.1	44.6	53.1	50.6	81.4	-3.1	-16.7	12.8	1.0	0.3	-0.9	-4.3											
Me2CHCO2H_3		-3.0	-2.4	-1.9	11.4	-5.1	-3.8	-16.2	7.9	-4.5	-6.6	-9.4	-0.1	-4.6	-1.0	0.7	-6.8	1.3	6.4	2.5	1.8	1.7			
-0.2	-2.5	-3.3	-2.5	-2.1	5.0	0.8	-8.0	3.7	0.1	5.4	0.9	-2.1	0.3	7.4	-0.3	2.5	-0.4	3.0	1.0	2.0	-2.3	1.3	39.8		
-3.9	10.9	58.8	-0.6	15.0	6.6	-3.8	1.5	28.2	7.0	8.4	35.3	-0.3	20.4	36.8	-1.8	-3.1	17.8	-0.5	-62.8	-7.8	98.9	108.3	-54.9		
103.2	86.4	-55.3	75.7	79.8	-15.6	7.6	72.7	18.8	32.4	84.7	-16.9	57.5	66.1	-7.1	-0.4	28.5	113.7	5.6	3.9	-3.1	22.4	28.6	12.3		
118.4	89.7	62.8	9.4	47.2	55.8	48.1	79.5	-8.4	-20.2	13.5	4.0	4.8	0.7	-1.5											
Me2CHCO2H_Avg		-1.1	-0.9	-0.5	13.0	-2.6	-1.1	-11.6	9.4	-2.0	-3.5	-5.1	4.1	-0.6	0.9	2.2	-3.5	3.8	11.7	2.9	2.7				
2.7	1.3	-0.6	-0.1	1.0	-1.3	7.4	2.8	-6.7	5.6	2.6	6.7	3.3	-0.2	3.2	9.8	0.2	2.2	0.8	4.9	4.1	3.6	-2.1	0.1		
39.1	-2.9	11.8	64.2	0.5	14.0	6.0	-2.5	1.5	26.8	7.1	9.0	32.7	0.7	19.8	38.7	-2.2	-5.6	15.4	-1.1	-62.7	-8.4	98.4	107.1		
-56.9	101.2	86.1	-58.9	74.2	78.2	-16.7	8.9	71.4	17.3	34.5	82.9	-17.5	58.8	66.7	-9.6	-1.2	26.3	109.7	3.8	2.7	-3.8	20.8	27.7		
12.5	114.4	85.5	59.4	9.1	45.4	54.7	50.6	80.7	-5.6	-17.1	11.3	2.7	2.1	-0.7	-3.4										
formicacid_1		-1.7	-0.6	1.4	-1.5	-4.8	1.3	-9.4	-6.5	2.7	-7.5	-3.2	-2.1	-0.9	-1.4	1.3	-1.1	0.6	4.9	1.2	-0.5	-2.6			
-2.9	-0.9	0.3	-6.2	-6.6	-4.4	1.6	-0.2	1.3	-1.0	-0.4	-2.8	-0.8	0.8	5.8	-3.7	-11.2	-14.7	-1.3	-5.3	-5.6	-6.0	-4.5	8.2		
-21.3	-32.1	29.6	-0.5	3.6	5.5	-1.2	-12.4	-0.9	3.9	1.4	10.2	-2.5	4.3	19.8	-11.3	-35.0	29.6	-15.8	-95.5	0.0	90.1	97.1	-64.5		
108.6	84.2	-70.7	69.7	71.1	-16.7	10.2	69.0	14.3	34.0	61.1	-24.7	85.4	58.0	-30.5	1.7	35.5	62.8	0.0	-8.9	0.4	19.1	22.5	10.2		
84.2	61.5	43.3	7.3	26.9	36.3	33.2	83.8	72.1	-20.3	17.7	7.6	4.5	-38.1	20.6											
formicacid_2		-1.6	-0.9	0.2	0.4	-4.4	3.5	-6.7	-5.1	5.9	-1.6	-1.1	3.5	2.9	-0.4	3.4	-6.3	-6.4	-6.9	0.7	1.7	-2.4			
-3.0	-1.9	3.7	-8.1	-6.0	-3.0	-2.1	-3.7	1.1	-2.4	-1.9	-5.2	-4.8	-1.2	0.2	-3.6	-10.7	-6.2	-4.1	-3.3	-3.5	-5.0	-4.7	16.6		
-16.9	-23.6	27.1	-1.8	0.3	2.9	-5.2	-10.6	2.9	5.2	6.0	16.0	-0.6	7.7	25.3	-11.7	-33.2	24.4	-12.6	-81.2	-4.8	86.2	92.3	-65.4		
100.6	79.7	-72.0	71.8	71.4	-15.0	10.3	69.6	13.6	33.2	67.8	-23.8	82.2	67.8	-29.6	1.0	32.4	79.1	0.3	-8.6	1.7	18.5	23.6	7.1		
75.0	57.0	35.8	4.1	25.2	34.2	26.4	72.8	62.3	-19.8	14.8	1.6	1.1	-32.7	19.7											
formicacid_3		-4.4	-2.4	-0.7	0.1	-3.2	2.1	-6.1	-1.4	6.9	-2.0	-0.4	6.0	3.9	2.7	4.8	0.1	3.9	6.6	1.6	1.8	-2.6			
3.3	2.3	9.6	-0.8	-0.1	3.6	-0.1	0.6	1.3	-0.7	2.4	-3.5	-0.2	3.1	2.7	0.0	-8.8	-5.7	1.5	-1.3	0.2	-1.0	1.1	12.1		
-16.3	-27.1	27.7	0.2	1.7	-1.1	1.5	-13.9	-1.5	5.0	1.6	11.7	-0.3	0.8	13.6	-12.3	-37.8	30.8	-13.3	-101.2	1.0	88.9	96.6			
-71.1	106.8	84.5	-79.8	67.9	67.8	-17.8	6.1	63.7	8.6	28.8	57.8	-29.2	79.2	53.0	-30.3	-0.2	31.3	63.7	-2.3	-11.9	-3.5	15.0	19.5		
formicacid_Avg		-2.5	-1.3	0.3	-0.3	-4.1	2.3	-7.4	-4.3	5.2	-3.7	-1.6	2.5	2.0	0.3	3.1	-2.4	-0.6	1.5	1.2	1.0	-2.5			
-0.9	-0.2	4.5	-5.0	-4.2	-1.3	-0.2	-1.1	1.2	-1.4	0.0	-3.9	-1.9	0.9	2.9	-2.4	-10.3	-8.8	-1.3	-3.3	-3.0	-4.0	-2.7	12.3		
-18.2	-27.6	28.1	-0.7	1.9	2.5	-1.6	-12.3	0.2	4.7	3.0	12.7	-1.1	4.3	19.6	-11.8	-35.3	28.2	-13.9	-92.7	-1.2	88.4	95.3	-67.0		
105.3	82.8	-74.2	69.8	70.1	-16.5	8.9	67.4	12.2	32.0	62.3	-25.9	82.3	59.6	-30.2	0.8	33.1	68.5	-0.7	-9.8	-0.4	17.5	21.9	8.2		
Cl3CCO2H_1		-12.3	-26.5	13.8	-54.1	13.8	-54.9	-60.3	9.5	-70.5	-25.9	-10.3	-38.6	0.2	-2.4	10.0	0.9	-0.1	6.3	11.6	-6.8	-7.1			
-41.2	-11.5	-14.2	-5.4	-15.4	-6.7	1.5	28.5	1.7	-6.8	-2.7	-17.9	-53.4	-7.0	-14.4	-15.6	14.0	0.1	-4.3	-2.3	-7.2	-3.0	-13.1	19.2		
-89.2	-130.0	26.4	-9.2	-23.3	14.3	-2.7	-87.1	0.1	4.2	-14.8	41.6	-26.8	-25.0	82.0	-16.5	-42.5	51.0	-25.0	-131.1	34.1	93.9				
27.6	-29.3	110.7	38.3	-34.5	86.9	93.5	-12.2	-119.1	-	-43.3	53.0	28.3	0.2	5.3	90.1	-28.5	61.5	0.4	29.2	16.3	-9.7	-67.2	31.0		
16.0	19.0	-3.3	92.0	60.5	28.8	0.5	24.7	36.7	32.3	86.9	68.5	-30.9	6.6	-3.1	-4.0	-78.3	10.9								
Cl3CCO2H_2		-3.3	-13.9	20.1	-48.2	19.4	-50.9	-54.7	20.4	-68.1	-20.4	-4.6	-35.6	4.8	2.5	15.7	8.1	10.1	13.1	13.3	-3.6	-5.1			
-41.1	-5.4	-8.9	-4.9	-13.4	-2.6	11.1	36.6	4.4	-7.6	-2.7	-18.7	-53.4	-2.4	-11.6	-16.7	1.3	-1.1	-10.5	-7.5	-12.9	-12.1	-23.5	11.3		
-96.2	-128.3	26.4	-16.7	-28.0	15.0	-8.5	-94.1	-1.6	1.8	-12.0	32.6	-26.7	-26.3	69.6	-18.8	-43.6	47.2	-30.9	-124.1	32.0	88.3				
18.9	-37.6	109.4	31.6	-43.9	84.9	95.0	-8.2	-113.3	-	-43.0	52.6	23.9	0.6	6.3	85.9	-18.6	69.8	-2.7	26.6	17.3	-13.2	-66.5	27.9		
17.3	20.6	-1.9	102.9	71.9	37.3	3.8	28.8	39.7	39.8	97.8	77.9	-27.0	10.5	2.8	-9.5	-78.7	7.5								
Cl3CCO2H_3		1.1	-12.3	26.6	-48.0	20.4	-50.8	-48.3	24.7	-61.7	-7.9	-4.9	-11.7	3.1	2.4	13.9	2.8	3.9	8.5	12.7	-6.0	-6.6			
-37.5	-3.2	-11.5	-0.3	-10.7	0.2	-1.1	28.3	-0.8	-5.7	-1.8	-18.8	-53.1	-5.4	-16.4	-9.5	-10.1	-6.2	-7.2	-6.9	-5.4	-5.6	-12.7	16.6		
-94.1	-135.9	20.7	-4.8	-21.0	13.2	-2.8	-86.9	1.7	2.1	-9.7	29.4	-17.8	-19.9	52.6	-16.6	-49.0	49.6	-25.7	-135.4	36.9	93.0				
27.3	-32.0	111.9	40.6	-37.1	83.0	88.9	-14.1	-114.3	-	-45.8	52.6	25.4	-2.9	8.2	89.0	-36.9	66.4	0.1	29.4	16.4	-6.6	-60.8	23.8		
15.6	20.4	0.9	86.9	60.5	32.2	1.6	24.5	37.7	32.2	83.1	70.1	-29.6	10.2	0.1	-5.3	-97.4	4.0								
Cl3CCO2H_Avg		-4.9	-17.6	20.1	-50.1	17.9	-52.2	-54.4	18.2	-66.8	-18.1	-6.6	-28.6	2.7	0.8	13.2	3.9	4.7	9.3	12.5	-5.5	-6.3			
-39.9	-6.7	-11.6	-3.5	-13.2	-3.0	3.8	31.1	1.8	-6.7	-2.4	-18.5	-53.3	-4.9	-14.1	-13.9	1.8	-2.4	-7.3	-5.6	-8.5	-6.9	-16.4	15.7		
-93.2	-131.4	24.5	-10.2	-24.1	14.2	-4.7	-89.3	0.1	2.7	-12.2	34.5	-23.8	-23.7	68.1	-17.3	-45.0	49.3	-27.2	-130.2	34.3	91.7				
24.6	-33.0	110.7	36.8	-38.5	84.9	92.4	-11.5	-115.6	-	-44.0	52.7	25.8	-1.1	6.6	88.3	-28.0	65.9	-0.7	28.4	16.7	-9.9	-64.8	27.6		
16.3	20.0	-1.5	93.9	64.3	32.8	2.0	26.0	38.0	34.8	89.3	72.2	-29.1	9.1	-0.1	-6.2	-84.8	7.4								
2Clpropionicacid_3		-1.0	1.2	1.1	8.3	4.0	-14.0	-7.9	7.2	-0.9	1.6	0.1	7.6	4.4	2.4	5.4	0.6	1.7	4.0	4.2	1.0	1.0			
-2.6	1.3	2.6	-1.1	1.8	2.0	3.3	-1.1	1.5	-7.9	1.5	4.0	-2.4	4.0	5.2	7.6	1.0	-12.8	-11.2	-2.6	-3.7	-2.2	-1.2	-4.0		
-9.6	-20.5	-34.9	19.2	0.7	5.8	7.3	1.4	-19.8	-10.4	1.6	-2.0	-6.8	-1.2	-9.3	2.1	-18.0	-36.7	29.8	-24.6	-111.8	12.3	97.4			
101.5	-84.8	115.9	88.0	-86.1	82.2	96.3	1.7	5.4	67.1	9.8	31.3														

CF3CO2H_2	6.4	2.0	34.2	-48.8	42.9	-38.5	-32.4	25.3	-54.1	-34.4	9.4	-13.4	-0.3	0.1	1.5	2.9	13.5	13.4	12.2	-4.0	-8.9			
	-8.7	-2.5	-5.9	2.0	-3.3	5.0	7.9	44.4	3.3	-0.8	4.3	-8.7	-43.3	2.0	33.8	6.2	14.5	-6.3	31.5	30.4	9.3	-2.4	-1.4	43.7
	-54.8	-93.7	19.9	-10.9	-20.7	53.9	-9.0	-56.2	10.1	5.6	5.9	56.8	-11.2	15.6	83.4	-13.7	-47.8	48.7	3.7	-118.2	27.1	65.5	38.3	
	-7.7	110.3	57.4	-16.7	60.0	72.9	-13.9	-133.3		-59.1	39.2	40.0	27.9	15.3	111.7	-16.1	48.5	-5.1	30.9	41.0	0.4	-41.0	17.4	43.2
	49.0	21.5	122.5	88.6	60.5	10.1	43.9	55.0	48.7	101.4	77.9	-22.0	14.8	-0.1	1.9	-82.0	3.7							
CF3CO2H_3	-8.0	-8.6	23.8	-58.9	34.3	-40.1	-40.1	17.7	-56.9	-43.7	6.6	-21.6	-5.4	-5.8	-1.3	-4.6	6.9	11.8	6.2	-7.5	-8.8			
	-12.8	-5.3	-7.2	-2.3	-5.5	5.7	16.4	45.1	8.1	0.0	4.4	-5.6	-37.6	4.9	38.2	4.4	10.6	-4.8	27.6	26.7	13.6	-2.9	-0.3	33.2
	-63.9	-108.9	18.3	-7.9	-16.1	50.7	0.6	-45.0	14.0	5.5	7.6	62.4	-8.0	13.2	69.5	-14.4	-49.6	53.7	7.4	-115.5	29.6	76.4		
	47.3	3.2	116.4	67.5	-15.5	62.3	75.6	-9.9	-131.6		-55.5	41.8	42.0	26.3	16.2	109.2	-26.1	50.3	-0.1	35.5	38.6	3.0	-30.0	12.7
	43.3	48.1	24.8	115.1	188.0	58.6	11.3	46.0	57.9	37.4	92.4	74.6	-25.9	15.5	3.0	1.6	-87.8	1.2						
CF3CO2H_Avg	0.9	-1.8	29.7	-51.6	39.0	-37.9	-35.1	21.9	-54.6	-38.0	9.2	-15.3	-1.9	-1.6	1.3	0.9	11.9	14.2	9.7	-4.9	-8.3			
	-9.7	-3.5	-6.9	-0.7	-4.1	6.0	14.5	48.3	6.6	-0.2	5.1	-7.0	-40.4	3.5	35.4	4.5	13.5	-6.1	29.2	27.6	10.3	-2.8	-0.5	37.6
	-60.6	-106.1	15.2	-9.4	-18.9	52.5	-3.9	-50.5	10.5	4.9	7.5	59.6	-9.5	14.1	78.2	-13.1	-49.2	51.0	5.0	-116.4	27.7	67.9		
	40.4	-4.4	110.9	60.0	-18.5	61.5	75.0	-12.3	-130.9		-58.0	41.1	40.1	26.6	12.8	108.2	-21.5	46.7	-3.2	31.9	38.2	2.3	-38.3	15.1
	43.1	48.5	23.3	116.3	85.7	57.4	10.5	43.5	56.3	41.6	94.8	75.8	-24.0	14.3	0.1	1.8	-85.1	1.3						
propionicacid_1	1.1	2.4	4.5	-5.4	1.6	2.9	-10.3	4.2	-3.3	-3.5	3.8	-1.8	-4.0	1.6	2.6	0.6	2.2	2.0	3.5	2.3	2.9			
	1.1	-0.2	1.9	-2.9	-4.0	-2.0	-4.0	-5.8	-2.3	3.3	3.0	2.0	1.2	0.9	3.7	0.2	-1.8	6.5	13.6	20.3	20.5	-0.4	0.6	22.2
	-6.9	1.5	16.4	-1.6	11.2	10.0	-1.9	-6.7	7.3	4.0	5.2	17.0	0.2	7.9	18.4	-2.0	-15.1	16.7	-0.5	-89.1	-0.3	106.2	117.5	-66.0
	107.6	91.6	-71.8	100.8	107.2	-2.6	8.8	98.1	25.9	26.6	81.1	-7.0	100.5	122.5	-13.5	0.6	33.3	129.4	0.8	-3.7	-1.1	28.9	43.1	20.0
	121.2	82.6	63.1	6.1	42.8	63.9	64.7	116.3	46.7	-16.1	18.2	1.7	6.4	-12.6	2.7									
propionicacid_2	-1.3	-0.9	1.7	-6.1	0.8	0.2	-7.3	5.9	-0.2	-3.8	0.1	-2.6	-5.5	2.5	0.7	-0.1	1.9	3.1	1.1	1.2	0.9			
	-3.0	-2.9	-3.2	-2.5	-2.4	-2.3	-0.4	-0.6	-0.1	2.5	2.8	3.1	-1.5	-0.4	2.8	-2.1	-6.1	-7.1	5.1	14.0	8.8	-5.5	-4.3	14.1
	-5.6	1.8	14.7	-2.1	12.7	8.4	-1.8	-5.6	2.5	2.6	1.0	15.2	-3.6	-1.7	10.2	-9.2	-11.5	8.6	-2.9	-87.6	-6.7	109.2	121.0	-64.1
	105.2	92.2	-62.6	104.0	110.3	1.3	15.9	99.5	24.3	32.3	72.9	-11.6	106.9	112.0	-19.3	1.5	37.9	117.2	4.3	-5.4	-0.6	32.6	48.1	20.6
	142.3	98.3	80.2	8.9	45.3	63.1	77.3	119.9	34.0	-19.7	15.3	6.3	4.6	-14.3	-0.4									
propionicacid_3	-1.3	-0.4	1.6	-4.2	2.6	1.8	-4.2	7.6	2.9	0.7	2.8	3.2	0.5	3.3	3.1	3.0	4.6	2.8	1.8	1.6	1.5			
	1.6	-2.3	-0.3	1.1	-0.1	2.2	1.6	-0.4	1.2	5.2	5.6	5.0	1.4	0.2	1.1	-0.6	-5.2	-3.7	10.3	18.3	15.4	-0.6	0.7	18.8
	0.1	4.7	15.0	-0.2	12.0	9.1	-1.0	-5.2	7.0	2.5	3.1	16.1	0.4	1.2	11.0	-7.6	-12.4	11.5	-1.8	-87.5	-7.0	105.0	115.5	-69.9
	102.1	88.5	-71.9	91.2	98.4	-2.3	13.1	85.1	17.7	28.3	64.9	-15.0	98.4	106.0	-25.4	-2.6	32.5	111.2	0.9	-9.5	1.6	26.3	36.2	15.5
propionicacid_Avg	-1.3	-0.6	1.6	-5.2	1.7	1.0	-5.8	6.7	1.4	-1.6	1.5	0.3	-2.5	2.9	1.9	1.4	3.3	3.0	1.4	1.4	1.4			
	1.2	-0.7	-2.6	-1.8	-0.7	-1.3	-0.1	0.6	-0.5	0.6	3.9	4.2	4.1	-0.1	-0.1	2.0	-1.3	-5.7	-5.4	7.7	16.1	12.1	-3.0	-1.8
	16.5	-2.7	3.2	14.8	-1.1	12.4	8.7	-1.4	-5.4	4.8	2.5	2.1	15.7	-1.6	-0.2	10.6	-8.4	-11.9	10.0	-2.3	-87.5	-6.8	107.1	118.2
	-67.0	103.7	90.4	-67.3	97.6	104.3	-0.5	14.5	92.3	21.0	30.3	68.9	-13.3	102.7	109.0	-22.3	0.6	35.2	114.2	2.6	-7.4	0.5	29.5	42.1
	18.1	135.0	90.9	73.7	6.1	41.7	60.1	71.0	114.8	30.8	-20.2	12.4	3.1	2.6	-15.8	-3.9								
aceticacid_1	-5.3	-5.1	-3.4	-1.9	-6.5	-2.6	-5.0	-6.1	-0.4	-5.9	-3.9	-1.4	0.0	-1.2	1.1	-2.7	-0.5	3.8	-0.1	-2.5	2.1			
	-0.8	-2.4	-0.3	-2.3	-2.1	3.5	0.7	0.5	2.7	-0.3	0.1	-1.7	-0.8	1.0	1.3	2.0	0.3	-8.6	6.9	-2.6	-3.8	-4.1	-2.3	-0.6
	0.3	13.5	60.9	-0.2	7.1	6.1	1.2	-2.2	2.3	6.3	4.6	2.2	1.7	2.5	4.8	-11.6	-19.7	14.1	19.4	-73.6	-14.2	83.0	87.0	-29.9
	104.9	80.3	-58.9	66.4	72.5	-14.2	12.3	84.4	16.1	41.4	90.8	-24.2	105.4	97.8	-23.9	1.4	37.4	105.9	5.4	-10.9	-2.2	35.6	44.6	19.1
	110.8	83.4	47.0	12.4	46.1	59.2	42.4	92.1	58.9	-23.7	14.1	9.4	2.7	-19.1	8.2									
aceticacid_2	-5.3	-3.1	-3.6	-1.0	-4.8	-2.1	-4.6	-3.4	-6.3	-4.8	-4.0	-4.3	-0.8	-1.4	1.9	-3.0	0.3	2.5	-2.2	-2.0	-0.2			
	-3.6	-5.9	-7.0	-5.7	-1.0	-1.9	-4.5	0.7	-4.2	-4.4	-3.7	-6.1	-5.2	-3.8	-5.6	-1.9	-11.0	1.3	-4.9	-7.5	-7.8	-7.4	-1.9	
	-10.3	4.0	52.3	-5.9	-3.3	0.6	-6.5	-9.1	-2.4	-2.7	-2.1	0.8	-6.9	-0.4	5.0	-17.0	-19.5	10.2	11.0	-70.6	-24.7	68.2	75.4	-34.6
	86.0	66.1	-62.0	62.7	68.8	-17.3	8.0	77.9	10.9	34.3	78.9	-24.7	97.4	85.8	-24.7	-5.6	29.7	98.0	1.1	-12.6	-3.0	38.9	47.1	22.6
	116.0	86.3	51.3	14.9	48.0	60.8	41.6	90.4	50.1	-20.1	14.8	11.6	2.2	-16.2	7.1									
aceticacid_3	0.8	2.0	2.9	3.9	1.0	1.6	0.2	0.9	4.9	-0.2	1.1	4.4	0.4	0.4	2.4	2.1	1.4	3.3	3.9	4.6	3.2	1.9		
	2.9	1.5	2.6	1.6	2.1	4.9	-0.4	0.6	1.4	0.5	1.6	1.1	0.2	3.8	3.0	2.7	0.0	-2.9	7.4	-1.4	-0.5	-3.7	0.4	
	-1.8	10.6	59.0	-0.3	4.8	-1.3	-0.4	-4.8	-2.5	2.8	1.5	1.6	-1.2	0.9	4.1	-17.4	-20.4	13.8	14.3	-76.5	-18.4	70.9	75.9	-36.5
	97.2	72.0	-64.0	60.2	67.1	-16.1	8.1	76.8	13.6	37.9	83.4	-24.5	104.1	90.5	-24.0	-6.7	30.1	99.9	0.0	-14.6	-4.2	36.0	41.3	18.4
	116.1	89.7	52.8	12.2	45.3	58.9	45.2	100.8	62.8	-21.3	15.4	8.2	0.2	-21.2	8.2									
aceticacid_Avg	-3.3	-2.1	-1.3	0.3	-3.5	-1.0	-3.1	-2.9	-0.6	-3.7	-2.3	-0.4	-0.1	0.0	1.7	-1.4	1.1	3.4	0.7	-0.4	1.3			
	-0.5	-2.3	-1.2	-3.6	-1.9	2.5	-0.5	-1.5	1.6	-1.3	-0.9	-1.4	-2.2	-0.2	0.1	-0.3	-0.6	-7.5	5.2	-3.0	-3.9	-5.2	-3.3	-0.4
	-3.9	9.4	57.4	-2.1	2.9	1.8	-1.9	-5.4	-0.9	2.1	1.3	1.5	-2.2	1.0	4.6	-15.3	-19.9	12.7	14.9	-73.6	-19.1	74.0	79.4	-33.7
	96.0	72.8	-61.6	63.1	69.5	-15.9	9.5	79.7	13.5	37.8	84.4	-24.5	102.3	91.4	-24.2	-3.6	32.4	101.3	2.2	-12.7	-3.1	36.8	44.3	20.1
	114.3	86.5	50.4	13.2	46.4	59.6	43.1	94.4	57.3	-21.7	14.8	9.8	1.7	-18.8	7.8									
pentanoicacid_1	-8.2	-4.3	-3.9	-4.4	-4.5	-4.2	-18.6	-1.4	-11.8	-13.4</td														

-3.1	-10.5	8.9	0.1	3.0	0.7	-0.9	-8.1	-0.9	7.2	2.6	4.9	-0.6	-1.3	6.3	-13.4	-34.8	22.1	-11.4	-97.3	-8.9	85.4	93.6	-49.1	
104.9	72.1	-49.1	81.4	86.8	-19.4	8.2	62.9	8.8	18.5	30.2	-15.8	59.6	6.6	-16.0	0.5	22.6	78.4	0.1	-18.1	-5.4	28.3	33.8	9.5	
128.2	297.8	63.3	4.1	28.8	42.3	46.4	107.7	86.4	-42.6	16.6	0.2	0.1	-10.3	-2.0										
CICH2CO2H_2	-0.2	0.0	0.3	1.8	1.4	6.2	-2.1	0.5	3.1	-0.4	1.9	4.3	2.5	2.8	5.5	-0.7	1.0	2.5	2.6	2.5	0.6			
1.4	-0.4	-1.1	0.4	0.3	1.0	2.9	5.2	5.1	-3.5	5.2	2.7	-0.7	0.7	2.1	-12.5	-15.3	-15.1	-6.6	-5.1	-9.3	-7.4	-8.0	4.9	
-8.7	-13.2	4.5	-2.1	-1.3	1.8	-3.9	-12.1	-1.4	-6.3	-10.8	-1.5	-6.8	-9.7	2.8	-17.5	-29.9	11.7	-14.3	-91.3	-17.5	79.4	87.7	-55.9	
105.2	271.9	-54.5	73.3	80.5	-25.0	4.8	54.7	4.2	15.2	34.7	-15.3	53.8	16.5	-18.6	-2.2	19.7	88.8	-0.3	-21.5	-5.9	23.6	30.7	9.0	
126.3	100.4	59.2	2.6	31.5	46.0	44.1	106.6	85.3	-44.4	12.1	-0.2	-1.5	-7.8	-1.3										
CICH2CO2H_3	-1.6	0.0	-1.9	-2.9	-0.8	3.9	-5.1	-3.4	-0.2	-3.6	-0.9	-1.6	1.7	3.2	4.8	-2.2	2.2	3.3	4.9	4.7	2.7			
-1.3	-0.5	-0.1	-2.4	-4.3	-0.9	-0.8	-1.0	0.2	-1.5	4.9	-0.8	-1.3	1.2	0.5	-2.1	-18.8	-10.3	-6.4	-6.5	-4.3	-2.3	-6.2	6.4	
-4.3	-10.5	1.5	-0.5	-2.2	1.5	-5.3	-14.2	-7.5	-2.4	-4.7	-3.8	-3.2	-8.4	0.7	-12.0	-26.8	14.0	-7.3	-93.7	-19.7	88.6	100.0	-59.9	
106.6	75.5	-52.1	79.1	86.6	-20.8	6.7	64.3	2.8	20.4	47.6	-11.8	67.8	37.7	-25.8	-2.1	21.2	103.0	0.2	-19.9	-12.3	27.9	36.5	13.6	
128.7	102.2	62.2	6.5	34.0	47.4	43.1	105.3	86.4	-41.6	12.7	0.8	-2.8	-7.2	-1.1										
CICH2CO2H_Avg	-1.1	0.2	0.0	-1.3	0.0	4.7	-3.5	-1.5	1.7	-1.7	0.5	2.0	2.3	2.6	4.8	-1.0	2.3	4.3	3.1	2.7	-0.3			
0.1	0.3	0.1	-0.6	-1.3	0.6	1.4	2.8	2.9	-3.2	4.5	1.0	-0.8	1.0	0.9	-4.6	-18.1	-11.7	-5.2	-5.8	-5.2	-3.0	-5.0	6.7	
-5.4	-11.4	4.9	-0.9	-0.2	1.4	-3.4	-11.5	-3.3	-0.5	-4.3	-0.1	-3.6	-6.5	3.3	-14.3	-30.5	15.9	-11.0	-94.1	-15.4	84.4	93.8	-55.0	
105.5	73.2	-51.9	77.9	84.6	-21.7	6.6	60.7	5.3	18.0	37.5	-14.3	60.4	20.3	-20.2	-1.3	21.2	90.1	0.0	-19.8	-7.9	26.6	33.7	10.7	
127.7	100.1	61.6	4.4	31.5	45.2	44.5	106.5	86.0	-42.9	13.8	0.3	-1.4	-8.4	-1.4										
BrCH2CO2H_1	-0.6	4.7	2.3	-14.8	6.1	-13.8	-3.9	3.1	-6.7	-0.1	-3.4	-0.1	-0.9	-0.3	2.0	-6.1	-6.6	-4.5	9.9	4.9	-0.6			
0.6	5.5	4.3	0.4	-0.6	-0.7	12.6	20.0	2.0	-7.3	4.3	-2.7	-6.1	-3.1	-6.1	0.0	-29.4	-10.4	-11.2	-9.8	-9.6	-6.7	-5.9	17.6	
-18.3	-33.2	19.7	-1.1	-10.7	-6.7	-5.8	-24.4	-1.4	1.2	-2.1	3.4	-4.3	-7.9	9.3	-28.2	-54.1	23.2	-37.5	-133.1	-2.2	72.3	73.4		
-63.8	99.2	57.5	-58.0	76.6	84.5	-27.5	4.1	49.1	0.2	13.2	-2.4	-28.1	51.3	-46.1	-19.0	-7.0	14.4	9.9	-7.0	-30.4	-14.3	24.7	32.5	
9.7	114.5	90.8	52.3	-0.2	29.8	46.3	45.9	106.4	85.9	-53.4	8.9	0.1	-2.7	-33.8	-11.6									
BrCH2CO2H_2	-1.4	0.6	0.8	-7.4	-1.7	-8.2	-7.9	-3.6	-2.8	-6.9	-4.7	-0.7	-4.2	-2.0	0.9	-3.9	-0.2	7.0	3.0	-2.1	-4.7			
-1.2	-0.7	-2.7	-1.9	-2.5	3.0	2.4	3.5	1.4	-5.3	5.6	2.1	-6.4	-2.5	0.5	-2.1	-27.3	-9.9	-7.5	-8.6	-1.4	-3.7	-1.5	18.7	
-18.0	-28.0	20.9	-0.5	-1.4	4.5	-4.5	-19.7	7.2	4.2	0.3	7.4	-1.4	-3.2	8.2	-18.7	-43.2	29.9	-26.6	-117.7	6.5	81.4	85.5		
-44.0	104.1	69.0	-43.0	74.9	80.6	-20.9	5.3	54.3	5.4	17.4	15.6	-18.3	55.5	-24.2	-9.6	0.2	18.1	45.7	-3.5	-16.2	2.8	23.3	30.0	
8.0	125.5	97.8	61.9	3.6	31.5	43.8	44.6	107.4	84.9	-40.0	24.1	-0.9	2.5	-19.1	4.0									
BrCH2CO2H_3	-5.6	-0.7	-1.4	-8.8	-2.1	-5.1	-8.8	-3.0	-3.5	-8.2	-3.5	-3.2	-3.7	-2.1	2.7	-8.4	-3.7	2.1	5.0	3.3	-1.5			
-2.2	1.1	0.6	-1.4	-2.1	3.4	2.8	6.0	0.4	-5.5	6.2	1.8	-7.2	-0.3	2.9	-1.3	-22.6	-1.5	-9.1	-4.1	-5.1	-5.8	-5.3	17.8	
-14.8	-25.5	23.3	-0.7	-0.3	5.3	-3.3	-18.7	7.8	3.2	0.5	8.9	-1.8	-4.5	11.0	-20.9	-41.9	31.2	-23.5	-116.2	12.6	82.3	87.8		
-41.0	106.1	69.8	-37.8	78.8	89.2	-23.7	6.2	54.0	8.6	16.9	18.5	-15.7	58.2	-23.4	-8.0	0.2	21.0	36.1	-0.5	-12.9	3.3	22.2	31.4	
8.2	118.8	93.0	58.7	3.3	32.9	47.8	47.3	108.5	87.6	-46.1	21.0	-0.2	2.4	-23.5	3.9									
BrCH2CO2H_Avg	-2.5	1.5	0.6	-10.3	0.8	-9.0	-6.8	-1.2	-4.3	-5.1	-3.9	-1.4	-2.9	-1.5	1.9	-6.1	-3.5	1.5	6.0	2.0	-2.2			
-0.9	2.0	0.7	-1.0	-1.7	1.9	6.0	9.8	1.3	-6.0	5.4	0.4	-6.6	-2.0	-0.9	-1.2	-26.5	-7.3	-9.3	-7.5	-5.4	-5.4	-4.2	18.0	
-17.1	-28.9	21.3	-0.8	-4.1	1.0	-4.5	-20.9	4.5	2.9	-0.4	6.5	-2.5	-5.2	9.5	-22.6	-46.4	28.1	-29.2	-122.3	5.6	78.7	82.2		
-49.6	103.1	65.4	-46.2	76.8	84.8	-24.0	5.2	52.5	4.7	15.8	10.6	-20.7	55.0	-31.3	-12.2	-2.3	17.9	30.5	-3.7	-19.8	-2.7	23.4	31.3	
8.7	119.6	93.9	57.6	2.2	31.4	46.0	45.9	107.5	86.1	-46.5	18.0	-0.3	0.7	-25.5	-1.2									
Me3CCO2H_1	0.9	0.4	-1.0	0.5	-0.6	7.4	-9.1	0.5	-2.3	-7.3	-2.7	0.1	-0.9	-0.3	4.1	7.3	14.1	2.9	4.4	3.8				
-2.7	0.1	0.0	-1.8	-3.5	2.6	1.6	0.0	-0.1	1.1	3.4	2.7	-1.9	3.8	7.7	1.7	14.8	14.7	7.0	10.7	8.7	-6.8	-1.0	49.5	
-9.0	7.5	48.5	-2.5	7.7	10.1	-9.2	-0.5	42.2	4.1	6.0	46.3	-0.4	19.0	46.0	-1.9	2.4	7.6	-1.0	-58.0	-6.2	86.9	98.2	-32.5	
83.0	66.3	-26.6	77.1	79.1	-32.2	10.2	64.0	25.5	22.9	59.1	2.0	61.0	75.1	2.9	-2.6	27.4	118.1	3.1	1.8	1.0	30.1	36.8	14.3	
137.2	211.3	171.0	9.3	33.7	40.1	51.5	52.5	10.7	-4.2	14.0	6.6	6.8	-3.3	-14.3										
Me3CCO2H_2	-1.2	2.7	3.8	2.6	0.6	10.9	-8.0	3.3	1.7	-1.8	5.4	10.6	4.8	6.7	7.6	6.3	10.6	14.1	3.9	4.8	2.7			
2.0	1.7	3.4	1.7	0.6	7.6	2.9	1.0	0.1	6.6	7.8	7.2	3.2	10.0	14.2	0.4	12.2	15.4	6.9	10.0	10.3	-2.8	3.2	59.8	
-1.6	12.3	54.3	0.1	13.5	7.4	0.2	9.5	51.3	2.7	7.6	52.3	0.1	18.9	49.0	-0.3	-2.3	3.4	-0.4	-61.0	-11.1	88.9	100.9	-36.4	
87.8	70.7	-30.5	80.9	82.2	-32.3	6.3	69.2	24.9	19.9	61.9	-3.5	61.0	76.7	-6.0	1.1	20.9	121.3	-0.5	2.4	-5.3	32.3	44.0	18.9	
136.2	211.1	77.0	7.0	29.6	39.6	48.1	48.6	8.9	-5.5	7.5	1.2	5.7	-7.3	-18.5										
Me3CCO2H_3	-4.6	-2.2	-1.8	4.0	1.9	12.1	-7.9	1.6	-2.0	-2.8	3.7	7.8	5.4	10.0	6.6	5.2	9.7	8.9	5.9	8.6	7.1			
1.2	14.4	22.1	3.1	1.5	7.2	3.1	2.2	1.4	5.1	8.0	7.1	3.7	9.8	12.7	1.1	13.1	17.3	6.9	13.2	14.0	-3.4	5.2	62.1	
-1.9	11.7	54.1	1.1	12.5	10.4	-0.4	10.6	51.0	2.4	8.6	53.1	0.6	21.0	44.1	1.0	3.2	5.5	0.3	-59.5	-9.3	89.9	103.6	-34.0	
90.5	72.2	-30.8	77.8	82.2	-25.4	6.6	67.6	28.4	21.0	59.6	0.5	59.8	73.6	1.0	-3.3	24.1	118.5	1.1	1.2	-0.1	27.6	35.2	9.7	
131.4	109.2	65.5	2.8	31.9	42.5	41.5	44.4	8.7	-7.6	8.2	1.3	2.3	-7.7	-17.5										
Me3CCO2H_Avg	-1.7	0.3	0.3	2.4	0.6	10.2	-8.3	1.8	-0.8	-4.0	2.2	6.1	3.1	6.4	5.8	5.2	9.2	12.4	4.3	5.9	4.5			
0.2	5.4	8.5	1.0	-0.5	5.8	2.5	1.1	0.5	4.3	6.4	5.7	1.7	7.9	11.5	1.1	13.4	15.8	6.9	11.3	11.0	-4.3	2.5	57.1	
-4.2	10.5	52.3	-0.4	11.2	9.3	-3.1	6.5	48.2	3.1	7.4	50.6	0.1	19.6	46.4	-0.4	1.1	5.5	-0.4	-59.5	-8.9	88.6	100.9	-34.3	
87.1	69.7	-29.3	78.6	81.2	-30.0	7.7	66.9	26.3	21.3	60.2	-0.3	60.6	75.2	-0.7	-1.6	24.1	119.3	1.3	1.8	-1.5	30.0	38.7	14.3	
134.9	111.4	69.0	6.4	31.8	40.7	47.0	48.5	9.4	-5.8	9.9	3.0	5.0	-6.1	-16.8										
perfluoroctanoicacid_1	6.0	7.1	43.1	-56.8	41.2	-32.4	-34.4	19.0	-34.9	-2.5	-13.0	0.4	3.8	2.9	6.1	19.3	25.5	25.5	19.4	5.7				
-1.9	-10.6	4.2	3.1	14.6	-7.5	3.5	-1.2	7.3	0.8	-0.9	20.1	4.2	-48.8	7.9	20.2	-8.3	-19.2	-18.1	4.4	-1.9	-2.6	-2.8		

86.2	68.0	4.0	108.3	55.8	-2.6	81.5	84.0	-24.9	-88.3	-14.4	87.7	16.6	-7.2	12.0	52.9	-68.4	58.0	0.1	19.5	48.7	1.7	-14.1	-1.1	
25.0	33.8	10.9	134.0	106.8	69.9	2.5	32.7	48.3	48.4	112.4	93.3	-61.6	19.1	1.7	-1.5	-116.0	-31.3							
hexanoicacid_1			-6.5	-4.7	-5.4	3.6	-3.1	-1.8	-5.4	-2.6	-2.7	-2.2	-8.4	0.7	-1.1	1.5	1.7	-1.2	-1.4	3.9	-1.9	-1.7	-2.7	
-3.2	-3.3	-2.3	-3.4	-5.0	0.5	-1.1	-0.6	-1.0	-4.1	1.0	0.6	-0.7	1.0	2.3	-4.1	3.7	-1.8	0.1	3.4	0.2	-4.1	-4.0	25.2	
-4.5	3.9	32.0	0.0	7.1	7.6	-2.5	0.1	22.6	0.1	2.2	29.9	-0.5	9.5	30.1	-1.8	-5.1	6.9	-1.3	-58.4	-7.9	92.0	104.6	-38.6	
93.9	75.4	-35.0	81.6	87.9	-23.9	6.5	60.8	23.7	20.9	60.9	-3.1	50.4	62.3	-0.3	-1.7	18.9	120.0	2.1	5.3	3.2	26.4	31.2	7.7	
127.5	98.0	68.6	7.3	38.2	53.2	54.0	85.1	-21.1	-10.5	10.2	5.0	4.8	-6.6	-20.6										
hexanoicacid_2			-2.6	-3.3	-4.0	0.4	-1.1	-2.3	-6.4	-3.0	-2.6	-7.5	-7.2	-2.3	-0.9	-0.3	-0.3	-11.2	-6.9	-6.4	1.4	1.4	-1.1	
-1.1	-0.9	-0.1	-3.4	-2.6	3.2	2.3	1.1	1.6	-2.7	0.4	0.1	-3.7	-1.5	0.7	-1.3	6.1	3.8	1.2	4.5	2.8	-4.1	-0.1	34.2	
-1.8	1.6	32.5	0.1	7.0	7.9	-1.4	0.3	19.8	1.5	3.2	24.0	0.7	8.0	20.8	-1.0	-4.5	8.1	-0.1	-55.1	-5.1	86.3	96.8	-35.9	
89.0	68.8	-34.4	72.8	76.0	-28.3	5.2	50.9	13.6	19.1	54.1	-6.7	48.0	58.4	-1.4	-0.5	17.9	115.6	0.8	0.7	-4.3	22.5	31.3	9.2	
128.6	102.6	68.5	9.1	38.3	52.4	53.4	82.4	-21.7	-7.9	6.7	0.7	-1.0	-8.3	-18.9										
hexanoicacid_3			-2.1	-2.8	-1.9	4.0	-1.3	1.3	-2.1	-1.3	0.7	-1.1	-2.6	4.8	1.4	3.2	4.4	-1.6	2.8	4.1	0.2	0.8	-1.1	
0.6	-1.0	0.0	0.3	-1.1	3.9	-2.5	-1.3	0.2	-2.3	3.7	3.3	-2.6	3.3	4.4	-1.2	3.9	4.9	2.2	1.7	3.5	-0.3	1.5	34.1	
-0.4	6.2	30.4	0.6	10.5	8.2	-1.8	3.6	28.5	0.6	3.5	25.9	-0.3	8.7	20.1	-0.8	-6.5	4.8	-0.6	-55.4	-5.8	84.6	99.3	-39.3	
89.1	70.3	-34.9	73.4	78.7	-29.7	1.8	52.9	15.1	11.8	51.7	-8.5	39.7	53.3	-2.8	1.3	7.3	115.7	-0.3	2.1	2.6	23.4	28.8	8.7	
122.9	97.1	62.7	1.4	26.8	37.9	47.1	83.5	-25.0	-10.5	3.8	0.6	0.1	-7.4	-16.7										
hexanoicacid_Avg			-3.7	-3.6	-3.7	2.7	-1.9	-0.9	-4.6	-2.3	-1.5	-3.6	-6.1	1.1	-0.2	1.5	1.9	-4.7	-1.8	0.6	-0.1	0.2		
-1.6	-1.2	-1.7	-0.8	-2.2	-2.9	2.5	-0.4	-0.2	0.3	-3.1	1.7	1.4	-2.3	0.9	2.5	-2.2	4.6	2.3	1.2	3.2	2.2	-2.8	-0.9	
31.2	-2.2	3.9	31.6	0.2	8.2	7.9	-1.9	1.4	23.6	0.7	3.0	26.6	0.0	8.7	23.6	-1.2	-5.3	6.6	-0.7	-56.3	-6.2	87.6	100.3	
-37.9	90.7	71.5	-34.8	75.9	80.9	-27.3	4.5	54.8	17.5	17.3	55.6	-6.1	46.1	58.0	-1.5	-0.3	14.7	117.1	0.9	2.7	0.5	24.1	30.4	
8.5	126.3	99.2	66.6	5.9	34.4	47.8	51.5	83.7	-22.6	-9.6	6.9	2.1	1.3	-7.4	-18.7									
nonanol 1			4.1	6.1	7.0	-1.0	7.2	-3.0	3.3	10.8	8.6	5.6	4.6	10.2	2.0	4.8	1.5	3.4	1.9	-5.2	-1.2	1.1	1.1	-7.9
-1.6	-2.6	-1.1	-0.4	1.6	-0.4	-1.3	3.5	-3.6	0.9	-2.2	1.9	2.1	2.7	-0.5	1.5	1.7	1.4	-3.1	5.8	-1.9	1.0	10.6	0.8	
2.4	6.3	-0.2	5.2	-0.3	-2.4	2.8	11.6	0.7	1.4	5.0	-0.2	2.6	5.2	0.1	0.7	3.5	-0.2	1.8	5.2	0.7	1.8	2.6	1.1	
0.7	0.9	-0.6	-0.9	3.2	-0.2	-1.3	-0.6	1.4	2.3	3.0	-2.4	-2.2	6.4	-0.6	6.2	0.6	0.2	3.6	0.8	5.0	9.8	6.3	4.2	
nonanol 2			1.3	0.4	0.6	-1.9	3.3	-7.4	1.3	2.7	-1.2	2.1	-2.3	2.8	1.2	1.9	0.9	4.9	-0.3	-5.9	0.3	0.7	-0.2	-5.7
0.8	-2.4	2.1	0.7	0.7	0.3	-1.4	3.0	2.4	4.4	2.7	-0.3	1.2	2.6	-0.6	3.1	2.0	1.1	-5.0	5.2	-0.4	1.2	17.8	-0.4	
3.6	10.4	0.8	3.9	0.2	-0.9	2.2	18.3	7.4	5.0	2.4	0.2	3.9	5.9	0.0	0.6	0.8	0.0	-2.3	1.5	-0.1	0.6	-3.1	1.5	
0.3	1.1	0.3	-0.5	2.8	0.3	-2.0	1.6	0.6	1.8	5.9	-3.7	-4.4	8.8	0.2	5.8	1.4	-0.4	4.6	0.6	0.2	0.0	1.0	7.4	
nonanol 3			1.5	1.7	1.6	-2.9	3.7	-6.4	-1.1	2.0	-2.4	0.0	-2.8	-0.9	-1.7	0.2	0.0	4.4	-1.8	-7.2	1.2	1.2	0.0	-4.7
0.8	-1.8	1.8	-0.1	0.1	-2.1	-1.9	-0.3	-1.4	2.9	-1.3	-0.4	0.9	0.7	0.3	0.9	2.6	0.2	-6.1	6.7	0.3	0.7	19.5	2.2	
3.7	12.2	-0.8	6.0	-0.7	-0.2	4.2	19.2	16.0	8.6	0.2	0.1	5.2	9.1	-0.4	1.0	3.7	0.1	1.3	6.8	0.5	0.6	-0.4	0.5	
0.3	-0.2	-1.5	-1.3	1.7	1.2	-2.9	1.6	0.6	2.4	1.9	-3.8	-5.8	6.4	0.2	3.1	-0.4	0.1	0.8	-2.3	0.3	0.8	2.7	12.7	
nonanol AVG			1.7	2.2	3.0	-3.0	4.5	-4.2	0.5	4.1	1.4	2.0	-1.1	3.0	0.5	1.8	0.8	3.5	-0.2	-5.9	0.2	0.8	0.2	
-6.0	-0.1	-1.7	0.6	0.1	1.4	-0.6	-1.7	1.8	-0.4	2.7	0.1	-0.1	1.4	1.9	-0.1	1.7	2.6	0.2	-5.9	7.5	-0.3	1.2	15.7	
0.9	3.5	9.2	-0.1	5.1	0.0	-0.8	3.4	16.2	10.9	6.6	1.0	1.4	5.6	6.0	0.2	1.0	2.6	-0.1	1.4	5.1	0.7	1.1	0.7	
0.9	0.7	1.5	-0.7	-0.4	2.4	0.7	-2.0	1.3	1.2	2.2	3.8	-3.7	-4.0	7.4	0.1	4.9	1.2	0.1	2.8	0.1	1.5	3.3	3.3	
7.5	15.1	12.3	0.0	0.0	3.5	6.1	-9.8	5.6	2.3	1.4	2.1	1.1	-0.8											
butanol 1			0.1	-2.1	1.1	-7.3	6.6	-8.2	-7.3	6.6	0.7	-7.7	-11.4	-2.1	-0.6	-0.6	0.5	2.0	1.5	-2.5	1.7	1.5	-2.0	-3.5
1.5	2.4	-0.2	-0.2	1.6	-4.0	-4.5	-1.9	1.0	3.3	0.9	1.2	2.5	5.0	0.2	12.7	-1.5	12.8	8.8	-3.0	-0.6	4.0	-2.5		
0.3	-16.4	-0.1	13.1	0.9	-2.3	6.3	8.5	-4.4	-4.1	-1.6	-1.0	0.5	-1.4	-2.1	-7.4	-2.5	-3.5	1.2	10.4	1.4	1.3	-5.3	5.8	
6.5	-0.2	-11.1	-11.3	-5.5	-0.6	2.0	-4.9	0.5	4.8	-7.0	2.7	-0.2	1.4	3.1	34.1	-8.1	1.3	9.7	-8.9	0.5	1.6	6.5	16.7	
14.9	26.0	1.2	-3.9	2.8	15.8	8.4	21.0	2.6	0.2	8.8	4.6	-8.3	-14.9											
butanol 2			-14.7	-11.2	-11.1	-12.8	0.6	-13.0	-15.0	-4.2	-10.8	-11.5	-9.2	-7.7	-4.0	-2.6	-0.1	0.6	-1.3	-2.9	-0.8	-1.8	-1.8	-11.8
-5.3	-3.2	-3.4	-5.8	-5.1	-3.1	-2.9	-5.3	-2.8	-2.5	-2.7	-3.2	-0.7	-6.2	10.0	-6.6	11.6	21.2	5.6	-7.8	-7.7	0.3	-5.9		
-4.2	-14.7	-1.2	7.1	1.2	-5.1	-1.2	-1.8	-4.7	-2.6	0.9	-2.8	-0.4	-0.5	-5.2	-7.4	-2.7	-6.2	-3.8	8.6	-3.2	-5.0	-6.8	-4.0	
-4.3	-6.8	-7.5	-8.3	0.6	3.0	3.6	-3.2	1.1	6.2	-1.6	1.3	1.9	2.6	0.6	22.5	-9.5	-0.1	5.4	-6.9	6.5	9.2	13.9	18.6	
17.5	34.9	6.2	-0.2	7.9	18.5	12.8	19.9	4.8	0.9	6.9	0.5	-8.8	-14.7											
butanol 3			-3.7	-5.9	-4.2	-11.5	2.0	-13.0	-12.3	-3.9	-8.9	-12.8	-15.0	-11.0	-6.5	-6.4	-5.2	-1.7	-2.6	-5.6	-0.4	-1.8	-1.9	-8.2
-3.7	-2.9	-4.4	-7.1	-4.9	-4.1	-4.8	-6.1	-6.6	-4.8	-4.5	-5.4	-3.8	-1.8	-1.2	6.4	-8.7	10.5	23.5	3.0	-6.7	-6.9	-2.5	-8.4	
-5.5	-23.4	-0.6	7.3	0.3	-6.6	-3.5	-3.3	-7.2	-6.1	-3.2	-2.7	-4.4	-1.5	-4.8	-10.1	-5.3	-4.2	-4.5	8.8	-3.6	-5.2	-9.6	-3.9	
-5.9	-7.9	-9.9	-11.1	-4.8	-2.5	-1.3	-6.0	-3.6	-0.9	-5.5	0.1	1.0	2.9	0.0	24.9	-9.3	0.6	6.1	-9.3	0.4	2.3	7.8	14.8	
11.2	26.5	1.4	-6.1	3.4	15.6	10.9	18.2	5.4	0.1	8.3	4.7	-7.8	-15.1											
butanol AVG			-6.1	-6.4	-4.7	-10.5	3.1	-11.4	-11.5	-0.5	-6.4	-10.6	-11.9	-6.9	-3.7	-3.2	-1.6	0.3	-0.8	-3.7	0.2	-0.7	-1.9	
-7.9	-2.5	-1.3	-2.6	-4.4	-2.8	-3.7	-4.1	-3.6	-3.6	-1.4	-2.0	-2.3	-1.5	0.8	-2.4	9.7	-5.6	11.6	20.9	5.8	-5.8	-5.1	0.6	
-5.6	-3.1	-18.2	-0.6																					

	AVG	-0.9	0.7	1.7	-1.1	3.5	-0.4	-0.1	4.5	2.0	0.0	1.1	1.3	-1.0	0.2	-0.2	2.1	0.8	-0.9	2.5	2.2	1.8			
dodecanol	0.6	1.8	3.2	0.5	1.5	2.4	4.2	-1.3	5.4	0.0	2.6	1.5	1.1	0.2	3.4	1.1	2.0	3.1	2.1	1.7	2.6	1.7	3.4	3.7	
	0.2	4.8	14.5	0.2	3.4	-0.3	0.4	3.7	5.0	0.5	1.0	2.5	0.4	2.9	1.3	0.7	2.7	1.3	-0.1	1.6	3.3	1.6	2.5	0.5	
	0.4	2.7	2.0	0.4	0.8	2.9	1.3	2.6	1.0	3.0	5.3	0.4	3.2	4.0	1.1	0.1	3.2	1.9	-0.6	1.4	2.5	2.7	2.2	2.9	
	3.7	5.3	6.2	0.9	1.2	1.6	-1.6	2.1	6.2	2.7	1.6	1.9	-0.1	2.9	2.4										
4-decanol	1		-1.4	-0.8	2.4	-4.3	6.5	-5.3	-2.8	1.0	0.5	-1.1	-6.4	4.1	-0.2	1.3	4.5	7.8	2.2	-4.4	2.4	3.0	3.4		
	-2.9	2.0	3.7	-2.0	-0.3	0.5	-2.8	-3.2	1.9	0.3	2.1	2.6	0.2	1.2	5.1	-0.4	22.2	10.1	6.1	15.1	7.2	-3.9	-4.8	10.4	
	-6.7	4.3	7.8	-0.4	8.2	11.4	-2.3	8.1	32.0	-4.2	-2.2	12.0	-0.7	3.1	16.7	-2.9	-0.6	5.5	-3.5	-2.3	3.1	-2.4	-0.7	1.3	
	-2.7	0.6	0.6	-2.8	0.2	2.4	-4.1	-1.3	1.9	-4.0	-0.1	2.3	-4.1	-3.0	5.2	-0.2	1.2	2.5	-0.4	13.5	12.7	9.7	18.0	16.5	
	5.5	8.9	9.3	-0.5	-2.8	9.3	0.9	2.6	8.0	7.5	4.5	7.6	2.3	3.9	7.8										
4-decanol	2		-5.9	-6.7	-2.0	-5.8	5.3	-5.7	-8.0	-1.0	-4.6	-5.2	-6.6	-0.5	0.0	2.2	0.4	5.8	-0.8	-2.9	2.3	3.7	2.9		
	-5.1	0.8	5.0	-1.3	0.4	-0.2	0.4	-0.5	1.1	2.9	4.5	3.9	1.7	0.2	3.6	0.5	24.6	16.7	12.8	20.4	13.3	-0.2	0.6	20.4	
	-0.4	10.9	16.6	-0.3	11.8	10.5	-0.7	12.5	37.6	1.1	2.7	19.6	0.5	13.8	25.3	3.1	3.3	6.3	0.0	3.3	5.2	-1.2	2.5	2.0	
	-0.4	1.6	1.4	1.9	3.4	4.7	3.0	1.0	2.9	3.9	4.3	4.9	-1.2	-1.7	4.7	-1.0	3.3	3.5	0.1	17.3	11.7	14.3	23.7	14.6	
	8.0	14.2	9.7	0.4	0.3	12.1	1.8	0.3	3.1	4.4	3.1	1.7	0.0	0.2	-0.9										
4-decanol	3		-0.3	-2.1	0.2	-5.2	6.4	-8.3	-3.2	0.9	-2.8	1.2	-4.0	2.1	0.6	1.8	1.0	6.9	-0.4	-5.9	3.3	4.5	3.3		
	-0.7	3.1	4.2	2.0	0.8	-0.6	0.3	-0.4	1.9	1.8	3.0	3.5	-0.4	0.0	1.2	0.7	22.7	10.5	9.4	18.2	9.3	0.2	1.3	14.8	
	-0.3	8.6	8.2	0.1	9.2	10.1	-0.3	7.5	25.4	-3.9	0.6	10.3	-0.3	8.5	18.4	-0.6	1.3	3.7	0.1	3.7	3.7	-0.2	0.2	2.2	
	-1.3	0.8	0.2	-0.2	1.8	1.4	-1.7	-4.2	1.9	-2.8	-3.4	3.0	-4.9	-7.5	5.3	-0.5	2.8	0.3	-0.1	13.1	12.4	6.9	12.2	7.2	
	4.9	9.7	6.2	-2.1	-7.7	11.2	0.3	-1.4	0.3	4.9	-0.6	-0.7	-0.1	1.3	1.7										
4-decanol	AVG	-2.5	-3.2	0.2	-5.1	6.1	-6.4	-4.7	0.3	-2.3	-1.7	-5.7	1.9	0.1	1.8	2.0	6.9	0.4	-4.4	2.7	3.7	3.2			
	-2.9	2.0	4.3	-0.5	0.3	-0.1	-0.7	-1.4	1.7	1.6	3.2	3.4	0.5	0.5	3.3	0.3	23.2	12.4	9.4	17.9	10.0	-1.3	-1.0	15.2	
	-2.5	7.9	10.9	-0.2	9.8	10.6	-1.1	9.4	31.7	-2.3	0.3	13.9	-0.2	8.5	20.1	-0.1	1.3	5.2	-1.1	1.5	4.0	-1.3	0.7	1.8	
	-1.5	1.0	0.7	-0.4	1.8	2.8	-1.0	-1.5	2.3	-1.0	0.2	3.4	-3.4	-4.1	5.1	-0.6	2.4	2.1	-0.1	14.6	12.3	10.3	18.0	12.8	
ethanol	1	-0.4	0.2	5.1	-3.8	3.4	-7.2	-6.2	3.5	-0.7	-3.9	-3.0	-0.3	-1.1	0.9	0.6	0.8	0.9	-2.2	1.2	0.8	2.2	-1.3		
	2.2	5.0	0.2	0.7	0.0	0.9	1.5	3.2	-1.4	2.0	1.0	1.7	1.3	1.6	0.5	19.5	6.7	11.8	22.5	14.4	-0.9	-1.0	13.6	0.3	
	-0.6	-32.3	-1.2	9.9	6.5	1.6	6.4	17.4	-1.0	0.4	13.2	-0.8	11.0	19.6	-0.4	0.4	1.7	0.1	-1.4	4.0	3.7	4.2	5.4	0.9	
	3.6	0.4	-0.7	-0.8	2.0	-0.6	3.0	2.4	2.7	6.2	2.9	4.7	5.3	3.8	0.2	6.8	3.1	1.5	17.3	5.8	16.8	24.3	17.4	15.2	
ethanol	3	-7.8	-6.2	-6.1	-8.5	-0.4	-10.9	-8.7	-0.8	-6.6	-8.0	-8.0	-3.7	-1.6	-2.7	0.4	-3.4	-1.8	-3.1	-0.6	-0.4	0.0	-4.4		
	-3.0	1.0	-4.7	-4.6	-5.1	-3.3	-3.7	-1.8	-5.4	-3.1	-4.5	-0.7	0.5	1.3	0.9	26.0	10.8	16.8	26.0	20.0	-4.5	-7.2	17.6	-6.5	
	-8.8	-30.8	-1.5	2.8	2.7	-1.8	7.9	28.4	2.6	3.9	29.6	-0.5	13.6	26.1	-4.0	-2.3	0.8	-0.4	-4.6	-0.4	2.0	1.3	-1.5	-0.3	
	3.4	1.4	2.0	2.6	4.9	4.7	7.9	1.9	5.9	9.1	2.8	8.7	10.6	5.7	0.6	5.1	1.7	4.0	10.7	-1.0	25.2	32.1	22.9	19.9	
ethanol	2	-4.5	-2.0	-0.6	-8.7	1.9	-8.2	-10.2	1.2	-4.6	-5.9	-3.4	-0.1	-0.2	1.3	2.7	2.1	3.0	-1.1	2.6	4.8	1.5	-2.2		
	2.1	3.5	-1.2	-0.6	0.9	1.0	2.4	1.9	-0.8	-0.4	-0.6	1.5	0.7	0.7	0.7	35.3	14.8	24.0	37.0	28.2	-0.9	1.4	22.2	0.3	
	-1.2	-35.5	-3.2	10.8	4.8	-3.4	7.2	22.8	-0.8	2.6	28.6	0.0	18.1	34.4	-1.4	2.5	6.6	-1.9	-1.5	4.7	6.4	5.2	-0.5	0.6	
	2.5	0.6	0.3	0.8	2.5	2.5	15.2	11.5	9.6	16.4	8.4	19.5	21.1	14.1	1.8	10.5	4.4	2.8	19.9	6.6	26.6	37.6	25.5	24.8	
ethanol	AVG	-4.2	-2.7	-0.5	-7.0	1.6	-8.8	-8.4	1.3	-4.0	-5.9	-4.8	-1.4	-1.0	-0.2	1.3	-0.2	0.7	-2.2	1.1	1.7	1.2			
	-2.7	0.4	3.2	-1.9	-1.5	-1.4	-0.5	0.1	1.1	-2.5	-0.5	-1.4	0.8	0.8	1.2	0.7	26.9	10.7	17.6	28.5	20.9	-2.1	-2.2	17.8	
	-2.0	-3.5	-32.9	-2.0	7.8	4.7	-1.2	7.2	22.9	0.3	2.3	23.8	-0.4	14.2	26.7	-1.9	0.2	3.0	-0.7	-2.5	2.8	4.0	3.6	1.2	
	0.4	3.1	0.8	0.5	0.9	3.1	2.2	8.7	5.3	6.1	10.6	4.7	11.0	12.3	7.9	0.9	7.5	3.1	2.8	16.0	3.8	22.9	31.3	22.0	
heptanol	1	-3.2	-1.6	1.7	-8.8	5.9	-13.6	-8.4	3.6	-8.4	-4.5	-4.0	-4.4	-0.7	1.5	-0.5	1.2	-0.5	-6.5	-3.2	-3.0	-4.8	-3.1		
	-1.3	4.3	0.0	-0.6	1.1	3.0	2.5	4.7	3.1	7.1	3.7	1.1	2.9	0.2	0.5	9.9	8.1	3.5	2.1	5.5	-1.9	1.7	16.6	1.0	
	14.0	20.2	-0.1	9.5	3.9	1.6	13.4	17.8	-3.3	0.6	12.9	0.6	6.5	6.6	0.7	3.5	4.2	8.6	6.3	11.9	4.3	6.3	7.7	3.7	
	7.0	3.5	1.1	3.2	5.9	1.1	11.6	2.6	4.9	14.3	4.6	6.2	7.0	7.7	0.4	9.2	3.4	2.1	5.5	0.3	3.4	6.3	9.4	27.2	
heptanol	2	-8.8	-7.0	-5.9	-10.1	5.6	-13.3	-8.7	1.4	-11.2	-6.3	-6.5	-5.0	-0.1	1.4	1.7	4.5	1.9	-1.0	1.6	1.6	0.2	-2.9		
	-0.8	0.7	-0.9	-0.3	-1.6	3.3	2.9	4.7	3.4	6.0	2.3	1.0	3.1	2.6	1.2	9.5	15.9	6.1	2.8	9.5	0.0	2.2	18.0	3.5	
	15.5	32.9	0.4	6.7	3.6	-1.3	10.7	18.5	5.3	7.5	13.4	-0.6	13.9	7.5	1.6	4.8	6.9	6.7	6.0	12.3	1.8	3.4	3.4	0.4	
	2.2	1.6	3.8	5.8	7.3	4.4	9.2	3.4	6.1	11.7	6.5	3.6	2.2	10.2	0.1	4.8	2.8	-0.4	3.3	0.8	4.1	3.8	7.2	31.0	
heptanol	3	1.5	-2.9	-2.5	-4.5	10.1	-11.7	-3.1	7.0	-6.3	-0.1	-2.2	0.7	0.5	-0.1	-2.7	4.3	-0.9	-10.1	3.7	1.7	-0.9	1.4		
	-1.5	1.6	0.6	0.3	2.9	0.9	2.6	2.4	3.2	2.6	-0.9	0.4	1.1	0.9	10.8	11.1	5.9	3.1	9.2	-0.7	2.7	16.5	1.6		
	14.7	26.5	-0.4	5.7	3.4	0.2	10.4	16.4	1.9	2.7	15.0	-0.3	10.8	7.6	-1.8	2.1	3.4	5.6	3.6	7.6	2.6	2.5	2.0	-1.5	
	2.6	0.8	0.5	2.9	3.1	0.2	5.9	-2.1	-0.1	8.8	3.3	0.9	-0.5	8.8	-0.9	4.2	0.2	-2.3	2.1	-1.6	1.4	1.1	5.2	24.9	
heptanol	4	-6.4	-5.4	-1.3	-10.3	6.8	-14.2	-13.2	2.7	-10.3	-9.6	-1.5	-3.7	-3.9	-1.6	-1.0	-2.5	-3.9	-5.5	5.0	4.5	5.7	-3.5		
	-1.6	7.6	0.3	0.6	3.3	0.1	0.6	4.7	2.3	2.9	2.3	-3.4	0.4	1.9	6.5	10.5	12.4	9.3	2.6	12.4	-0.6	6.5	21.5	2.5	

1.0	12.7	42.0	-0.1	1.8	5.5	-1.3	3.9	4.9	-1.2	-0.3	2.3	-0.2	3.2	-0.1	-1.7	0.6	1.5	3.1	-2.4	0.0	-0.7	0.3	0.3	
-1.6	0.0	0.0	-2.2	-0.4	0.4	-1.8	9.0	-0.3	2.6	9.2	-2.0	7.9	10.5	-4.2	-0.6	1.2	0.4	-2.9	-2.5	1.1	1.2	3.3	2.8	
12.7	13.6	12.7	-3.0	-3.5	0.0	-4.8	-0.6	3.5	-1.9	0.4	-1.3	-1.3	0.3	2.4										
2-decanol	1		-3.9	-4.0	0.0	-6.7	5.7	-14.5	-3.4	3.9	-3.7	-0.8	-2.0	0.9	-0.7	1.6	1.5	6.5	-1.7	-6.1	2.4	1.2	2.8	
0.8	-0.1	4.4	1.5	0.9	2.3	1.6	1.0	4.8	2.6	6.2	2.7	0.5	1.6	1.7	2.2	4.3	3.4	2.7	0.8	5.8	0.9	3.5	8.2	
3.9	17.0	49.7	-0.3	4.2	7.1	-0.4	6.1	5.5	1.6	2.5	6.8	0.0	5.4	0.4	0.8	2.2	3.5	6.1	0.1	1.0	0.2	1.9	0.8	
0.2	1.7	1.7	-0.4	-0.6	2.0	0.2	10.5	-0.6	3.8	11.2	-1.9	8.7	10.8	-2.0	0.2	3.2	2.5	-2.2	-1.0	3.3	3.7	5.4	6.6	
12.1	14.7	13.4	-0.5	-0.5	1.5	-2.1	0.6	7.1	-0.2	3.4	0.0	0.0	2.7	4.3										
2-decanol	2		-2.0	-2.8	-2.8	-8.5	4.7	-14.0	-2.5	2.7	-6.8	-3.2	-6.9	-2.0	-1.4	-1.7	-2.3	3.0	-4.5	-8.9	-1.2	-1.4	-1.4	
-2.8	-3.9	-1.2	-2.8	-2.7	-2.2	1.5	-2.1	5.1	-1.4	0.4	0.8	-1.9	-1.9	-1.3	-2.3	0.8	-1.1	-2.7	-1.8	-2.7	-1.9	-1.3	2.7	
-3.0	7.1	31.1	-0.1	-0.9	3.2	-4.1	1.3	5.2	-6.0	-3.4	-0.5	-0.8	1.2	0.1	-4.6	-1.2	-1.2	-2.2	-5.7	-0.6	-1.7	-1.4	-1.6	
-3.7	-2.0	-2.0	-3.7	-1.5	-2.0	-4.6	8.6	-1.0	-0.5	7.3	-3.2	8.4	11.8	-7.4	-2.1	-1.5	-1.4	-5.2	-5.7	-0.1	-1.9	0.5	-1.3	
10.2	12.0	8.4	-6.8	-5.1	-4.0	-7.4	-2.6	2.4	-6.3	-2.5	-4.8	-4.4	-2.3	0.7										
2-decanol	3		-6.3	-5.0	-4.6	-10.1	3.4	-12.5	-9.1	-0.4	-5.6	-4.5	-3.9	-3.9	-2.7	-1.4	0.6	2.0	-3.4	-8.7	0.4	0.4	-0.9	
-1.9	-0.9	3.3	-1.6	-1.1	0.2	-0.4	4.5	-0.6	1.2	0.7	-3.6	-2.2	-0.7	0.9	2.6	2.8	2.7	-0.3	3.1	0.5	-0.2	5.0		
0.2	11.6	40.5	-0.1	0.3	5.5	-0.8	2.1	3.1	-1.2	-1.6	-0.7	-0.3	1.7	-1.3	-3.1	0.6	1.7	3.0	-2.2	-1.2	-1.7	-0.6	0.1	
-2.2	-0.9	-2.1	-3.9	-1.3	-0.9	-3.5	6.4	-1.2	2.0	7.6	-3.5	6.1	8.9	-4.5	-0.6	-0.5	0.0	-2.6	-3.7	0.8	-1.3	1.5	0.0	
13.2	13.2	12.2	-5.1	-6.5	0.0	-7.1	-2.9	-0.4	-2.6	-2.2	-3.2	-1.7	-0.7	0.4										
3-decanol	1		-1.2	-2.0	-0.4	-7.8	4.1	-12.5	-7.4	-0.4	-5.3	-6.6	-2.5	-3.9	-2.4	-1.6	-1.7	3.8	-4.2	-10.0	1.9	0.5	-0.4	
-1.7	-4.2	2.4	-1.6	-4.3	-3.6	-0.5	-2.6	3.9	1.4	2.3	2.0	-2.6	0.9	1.4	-0.6	2.3	0.8	0.7	-0.6	0.5	-1.8	-3.1	5.3	
-2.0	8.0	34.6	-0.8	0.8	7.6	-1.9	2.8	4.2	-0.3	1.0	3.3	-0.4	3.8	2.9	-2.2	2.9	4.2	0.9	1.1	4.0	0.5	1.0	1.9	
-1.5	0.7	0.6	0.1	1.5	2.6	-0.8	-0.6	2.0	3.6	3.7	-0.5	-0.6	-3.9	7.7	-0.4	0.9	3.3	-0.9	0.6	1.9	1.9	3.3	4.4	
11.7	15.4	12.4	3.5	0.2	4.8	-2.7	4.0	9.1	4.2	4.1	4.9	-0.3	5.0	3.6										
3-decanol	2		-2.8	-1.4	1.2	-7.3	6.4	-7.8	-8.8	2.1	-0.5	-4.4	-2.8	-0.6	-2.9	0.7	-0.2	6.6	-2.6	-9.3	0.5	0.8	1.9	
0.4	0.7	5.4	0.3	-0.3	2.7	-0.5	-1.3	6.0	1.0	3.6	2.4	-3.6	1.1	3.6	1.8	1.6	3.2	2.5	-0.3	5.9	-1.8	1.8	7.8	
-2.4	13.0	41.6	-1.7	1.8	6.1	-4.1	3.5	5.2	0.6	0.8	1.2	-0.3	3.6	1.4	-1.6	3.3	3.3	0.1	1.4	5.5	-1.2	0.2	4.0	
-1.2	1.5	2.8	-1.9	-0.6	1.8	-2.3	-3.4	0.7	-0.5	3.6	1.9	-3.4	-4.8	9.4	0.4	3.6	0.9	-2.3	0.8	3.8	-0.8	1.4	4.2	
7.0	12.7	13.2	-0.5	-3.7	3.2	-4.9	1.2	5.9	3.5	3.5	2.2	0.7	4.9	6.9										
3-decanol	3		-0.6	-0.4	1.1	-3.7	8.7	-9.2	-5.1	4.2	-2.5	0.0	-3.4	0.4	-0.9	1.0	0.4	8.1	-0.4	-7.9	2.3	2.6	2.4	
2.7	1.1	8.9	3.1	1.1	3.2	2.7	0.4	8.8	4.1	6.6	5.9	0.5	2.4	3.3	0.2	2.7	1.9	1.9	-0.2	2.7	-1.0	3.2	6.9	
2.7	18.9	53.2	-0.4	3.4	5.5	-0.1	5.5	4.5	-0.1	0.6	3.2	0.6	4.2	0.8	1.1	1.3	1.3	2.0	2.4	0.7	-1.8	-0.7	2.0	
-1.8	-1.1	2.8	-2.8	-0.9	0.0	-0.8	-2.2	-1.0	0.3	1.2	1.7	-4.9	-6.9	4.1	-0.6	-0.1	1.5	-1.8	-0.1	-1.5	1.2	1.4	1.4	
10.8	15.3	13.6	-0.3	-1.6	3.4	-3.8	1.3	6.6	3.4	0.9	2.1	1.6	3.1	1.7										
3-decanol	AVG		-0.7	-1.7	0.1	-5.5	6.2	-10.2	-6.2	2.3	-2.4	-2.8	-2.6	-1.2	-1.6	-0.2	-0.6	5.1	-3.3	-11.6	1.9	1.5	0.9	
0.7	-0.7	4.9	0.6	-1.2	0.5	1.0	-1.5	5.4	2.1	3.6	2.7	-2.0	1.2	2.6	0.4	2.1	1.6	1.9	-0.6	2.6	-1.2	0.4	6.5	
-0.7	13.0	41.5	-0.7	1.5	5.8	-1.7	3.8	3.3	-0.5	0.2	2.8	-0.1	3.1	0.6	-1.3	2.0	2.3	0.1	0.8	2.2	-1.4	-0.2	1.6	
-1.6	0.0	1.4	-1.4	-0.3	0.9	-1.8	-2.6	-0.1	0.4	1.7	0.1	-3.9	-6.4	6.1	-0.1	0.9	1.5	-1.5	0.1	1.0	0.7	1.9	3.0	
benzyl alcohol	1		-1.3	-0.6	0.6	-6.7	7.1	-12.2	-5.4	5.2	-3.8	-2.6	-14.3	-4.2	-0.5	2.2	2.0	2.0	-0.7	-5.3	-0.8	-0.4	-2.8	
-1.5	0.1	-2.0	-0.1	-0.2	0.2	-2.6	-2.7	-1.7	-0.6	3.0	-2.5	1.1	1.8	2.5	0.8	-4.1	1.7	-1.8	1.8	-0.1	2.3	2.3		
-0.7	-1.8	-8.4	0.1	-0.7	-7.2	0.3	-0.3	-1.7	-1.3	0.1	-1.0	0.3	-3.6	-5.4	-3.3	-4.2	6.5	9.7	1.8	-1.1	-2.5	4.3	3.3	
-2.5	5.1	0.2	-3.5	-3.7	-0.5	0.5	3.4	-2.2	-0.5	5.0	-4.4	-1.2	-0.3	-4.9	0.3	8.1	-1.2	-1.8	-1.8	-3.0	7.2	1.9	5.1	
9.8	-5.8	20.7	3.8	3.5	-0.3	19.4	12.8	1.0	-2.6	3.7	5.0	0.2	-5.9	-3.6										
benzyl alcohol	2		0.3	1.2	2.3	-3.7	8.2	-8.1	-4.0	6.5	-2.8	-3.1	-10.8	-3.8	-1.8	1.9	5.1	-2.2	-1.5	-4.5	1.7	0.1	-3.4	
1.1	0.5	0.6	1.6	0.9	-0.5	1.3	1.6	0.1	-0.5	1.8	-3.0	-1.7	0.3	0.7	-0.1	-5.0	2.5	3.0	0.2	-3.4	-0.1	2.3	5.7	
-1.3	-2.0	-8.2	0.4	-3.7	-5.9	-0.6	-0.7	6.7	-3.2	-1.4	-1.0	0.3	-4.2	-4.9	-5.3	-4.6	2.8	0.8	0.5	-4.0	2.2	-0.3		
-4.6	2.1	-0.1	-2.7	-5.3	-3.4	-0.4	0.1	-1.2	-6.4	-0.2	-4.1	-4.4	-5.3	-1.4	0.0	5.6	-1.5	-1.6	-1.9	0.5	2.5	0.2	1.3	
11.1	-9.5	21.9	3.0	2.3	-0.9	20.1	13.0	0.3	-1.2	7.9	5.9	0.9	-6.0	1.6										
benzyl alcohol	3		2.4	-0.2	3.4	-3.2	7.2	-7.1	-3.5	5.2	-2.7	-1.0	-12.3	-2.4	1.1	1.5	3.5	0.1	-0.6	-2.2	0.2	-0.9	-3.0	
-0.4	-0.7	-1.1	0.8	-0.3	1.8	2.5	0.8	0.2	1.8	0.2	-1.1	1.4	2.1	1.0	-4.9	0.6	2.8	-0.4	0.1	0.8	0.8	-2.1		
1.0	-2.5	-11.8	0.3	-2.6	-3.4	0.3	1.0	2.8	-0.5	-0.1	2.0	0.9	-5.1	-4.9	-2.0	-5.8	8.2	4.9	-1.5	-5.5	-2.6	2.4	-0.8	
-3.7	3.4	-1.2	-2.4	-5.1	-2.6	2.1	5.6	-0.2	-1.5	4.8	-6.6	-4.0	-2.6	-4.6	0.7	3.6	-2.3	-0.8	-2.1	1.8	3.7	1.5	2.6	
10.5	-7.1	20.2	2.5	1.0	-2.8	12.9	5.3	1.3	-3.9	3.5	1.3	0.2	-7.0	-0.6										
benzyl alcohol	AVG		0.5	0.1	2.1	-4.5	7.5	-9.1	-4.3	5.6	-3.1	-2.2	-12.5	-3.5	-0.4	1.9	3.5	0.0	-1.0	-4.0	0.4	-0.4		
-3.1	-0.3	0.0	-0.8	0.1	0.5	0.4	-0.1	-0.5	0.2	1.7	-2.2	0.3	1.4	1.4	0.6	-4.7	0.9	2.5	-0.7	-0.5	0.2	1.8		
2.0	-0.3	-2.1	-9.4	0.3	-2.4	-5.5	0.0	0.0	2.6	-1.7	-0.5	0.0	0.5	-4.3	-5.1	-3.5	-4.9	5.8	5.1	0.3	-3.6	-3.8	3.0	
0.7	-3.6	3.6	-0.3	-2.9	-4.7	-2.2	0.7	3.0	-1.2	-2.8	3.2	-5.0	-3.2	-2.7	-3.6	0.3	5.8	-1.7	-1.4	-2.0	-0.3	4.4	1.2	
3.0	10.5	-7.5	20.9	3.1	2.3	-1.3	17.5	10.3	0.9	-2.6	5.0	4.1	0.4	-6.3	-0.8									
2-phenyl-1-propanol	AVG		0.7	0.5	2.3	-13.5	14.9	-13.8	-4.9	8.1	-7.3	2.6	5.1	-2.5	0.1	0.9</								

-26.5	3.4	5.4	-19.8	4.2	2.1	1.4	5.3	22.4	-2.1	14.4	33.4	-13.5	20.7	21.7	-8.3	0.1	5.6	-6.5	0.3	-2.2	-2.8	6.0	8.6
3.6	7.6	-5.4	29.4	-1.6	-4.5	-0.9	15.2	5.9	-8.0	-4.8	-6.1	-8.8	-3.1	-5.5	-7.2								
3,3-dimethyl-2-butanol	AVG		-3.9	-3.3	-1.9	-15.9	11.4	-10.3	-10.5	7.9	-3.9	-2.6	4.0	-5.7	-0.9	0.1	-0.7	1.9	-1.6	-6.5	2.2		
2.5	1.5	-5.8	-5.2	1.5	-1.9	-5.8	-3.1	-3.4	-4.4	-1.2	4.7	4.1	5.3	-0.1	-0.7	-1.0	-1.9	-2.6	3.9	1.2	14.1	13.1	-6.8
-4.6	25.0	-6.3	9.3	12.5	-1.1	11.2	0.2	-2.0	5.8	21.2	-5.6	2.5	24.9	-3.1	0.5	13.0	-3.2	1.3	-2.2	-2.2	-22.1	11.4	30.6
34.6	-29.4	17.0	22.1	-17.1	15.6	11.5	6.4	7.9	70.9	17.1	24.3	65.6	-1.4	78.1	92.2	-8.0	0.0	26.4	5.3	1.8	11.2	-1.0	0.0
15.1	14.6	25.3	19.9	36.6	-5.4	-4.5	24.3	7.5	12.0	11.4	1.5	6.0	4.0	2.4	-1.6	-6.8							
3,3-dimethyl-2-butanol	1		-3.9	-2.5	-0.1	-15.4	9.8	-10.7	-10.7	6.8	-2.2	-1.1	6.7	-3.6	-1.2	1.2	-0.4	1.4	-0.1	-5.3	2.4		
3.0	3.8	-6.7	-6.0	0.5	-1.8	-4.5	-1.7	-2.4	-3.6	-1.8	4.5	3.3	6.5	-1.7	-2.6	-1.9	-4.1	0.4	4.7	-0.6	13.2	12.6	-6.6
-2.2	24.7	-4.0	11.5	11.4	-3.5	12.1	-1.8	-4.3	5.1	21.4	-4.9	3.2	21.7	-2.2	2.3	14.6	-3.0	1.5	-2.1	-1.0	-21.8	9.3	34.2
38.8	-33.2	20.4	25.8	-18.4	17.0	12.7	10.8	10.2	74.0	19.5	24.6	66.3	-2.6	80.6	95.4	-12.0	0.2	31.5	2.3	1.3	13.9	-0.7	-0.4
14.5	14.8	24.0	20.2	37.5	-7.3	-7.7	22.1	4.8	12.1	10.0	0.0	4.0	-0.7	2.7	-0.4	-6.2							
3,3-dimethyl-2-butanol	2		-4.3	-4.5	-2.5	-14.8	11.0	-9.6	-9.7	4.7	-7.3	-1.7	1.9	-5.2	-0.1	0.5	-0.1	2.5	-1.1	-6.9	1.6		
2.1	-0.3	-5.8	-4.6	1.0	-1.7	-5.0	-1.8	-3.9	-3.1	0.5	6.5	5.8	6.9	2.2	0.5	0.1	-0.9	-0.7	7.3	2.6	17.4	14.5	-5.6
-3.8	28.4	-4.6	10.7	16.5	0.8	12.5	2.8	-0.4	6.2	19.9	-2.6	4.7	30.1	-3.1	1.9	17.2	-3.2	2.8	-1.5	-1.8	-19.1	15.3	28.1
31.6	-25.7	13.8	17.3	-16.2	17.6	15.5	10.7	9.4	74.2	22.4	25.9	67.3	3.8	76.2	90.0	-2.4	0.0	22.8	6.3	2.8	11.5	-1.4	1.4
15.8	14.1	26.9	22.1	39.4	-2.8	-2.4	26.5	8.3	10.7	12.6	1.1	6.5	5.5	2.6	-2.9	-9.3							
3,3-dimethyl-2-butanol	3		-3.5	-2.9	-3.0	-17.6	13.5	-10.5	-11.0	12.2	-2.1	-5.0	3.5	-8.2	-1.6	-1.3	-1.6	1.9	-3.7	-7.4	2.5		
2.5	1.0	-5.0	-5.0	2.9	-2.4	-8.0	-5.9	-4.0	-6.4	-2.2	3.1	3.3	2.5	-0.8	-0.1	-1.1	-0.6	-7.5	-0.2	1.5	11.9	12.2	-8.0
-7.8	22.0	-10.4	5.7	9.6	-0.7	9.0	-0.2	-1.3	6.0	22.2	-9.2	-0.5	23.0	-4.1	-2.8	7.3	-3.4	-0.4	-3.0	-3.8	-25.5	9.6	29.7
33.3	-29.3	16.7	23.4	-16.8	12.4	6.4	-2.3	4.2	64.5	9.5	22.3	63.3	-5.4	77.5	91.3	-9.7	-0.3	24.9	7.2	1.2	8.1	-0.8	-0.9
15.0	15.0	25.1	17.3	32.8	-6.1	-3.3	24.4	9.3	13.3	11.8	3.5	7.4	7.3	2.0	-1.4	-4.8							
1-decanol	1		1.7	1.6	3.3	-6.6	9.4	-8.8	-4.5	10.2	-5.8	-0.1	-3.0	-2.3	1.4	1.8	0.6	3.3	0.9	-6.5	1.8	1.9	-1.0
1.0	-0.3	5.0	3.2	1.5	5.3	3.5	2.1	7.5	2.8	5.5	3.3	2.7	4.0	4.0	0.5	6.6	13.9	1.5	4.1	5.8	1.5	5.0	17.5
3.3	9.2	13.0	-0.3	9.4	2.0	1.9	12.5	17.3	1.6	4.3	14.4	1.1	2.7	5.1	1.1	3.4	4.1	1.1	10.3	8.9	1.3	3.0	8.2
3.4	4.3	5.0	-0.8	0.7	4.0	-1.2	-8.5	3.0	-1.0	-1.4	7.3	-10.1	-8.8	10.6	1.1	3.3	3.1	0.4	5.3	1.1	-2.2	-3.1	4.3
0.8	3.7	12.6	2.0	0.7	5.4	2.8	3.9	6.0	4.4	3.8	-1.1	2.9	4.0	1.5									
1-decanol	2		2.2	1.5	1.0	-4.2	9.2	-8.2	-2.8	10.3	-7.2	0.4	-10.1	-4.8	0.2	-0.1	1.1	3.9	-0.4	-4.2	1.9	0.0	-0.1
2.8	-0.7	1.3	4.1	1.8	0.7	1.6	-0.8	8.3	3.5	4.0	3.9	2.0	2.5	3.9	-0.5	7.9	11.9	2.2	2.5	5.0	0.1	2.9	14.5
2.3	6.9	13.3	-0.1	5.2	2.2	1.0	9.7	19.2	0.5	3.5	15.9	1.2	1.4	6.4	2.0	2.8	3.2	0.6	7.7	6.7	0.4	0.8	3.9
1.7	2.0	2.3	4.5	5.5	5.8	1.3	-9.0	1.5	-1.4	-2.7	5.5	-11.2	-13.0	9.8	-0.1	1.0	3.4	-0.3	3.1	2.0	-3.6	-3.1	1.5
3.5	3.3	14.6	0.6	0.3	2.9	2.7	0.8	4.0	3.2	1.6	-0.1	0.5	3.8	5.0									
1-decanol	3		1.3	0.9	-0.3	-5.9	10.1	-7.0	-4.2	12.3	-7.0	0.1	-4.8	-2.0	1.1	1.2	2.8	2.1	-4.1	-10.1	2.2	1.7	1.6
3.0	-0.2	1.9	3.9	3.4	3.9	1.0	2.0	7.1	3.7	5.3	3.5	3.8	2.4	3.1	-0.8	8.8	11.1	2.5	3.7	4.3	0.8	3.9	14.2
2.6	8.1	12.7	0.3	4.5	2.5	2.2	7.3	14.6	3.2	4.2	7.6	0.5	3.4	4.2	4.2	3.5	2.8	0.7	9.1	7.3	1.5	1.6	6.3
1.9	1.8	4.1	3.9	4.6	4.5	1.1	-7.7	1.6	-0.3	-0.9	5.1	-11.6	-11.5	9.2	1.1	1.5	2.9	2.6	3.6	2.6	1.0	-1.6	-0.2
2.7	3.5	11.3	1.8	0.3	2.7	3.7	3.2	2.7	5.1	2.6	1.4	2.5	3.0	3.8									
1-decanol	AVG		1.5	1.1	1.4	-5.9	9.3	-9.2	-4.5	10.5	-7.2	0.1	-5.7	-3.4	0.7	0.9	1.2	3.3	-1.2	-6.8	1.8	0.9	0.0
1.8	-0.7	2.1	3.7	1.8	2.9	2.1	0.9	7.3	3.5	4.4	3.2	2.6	2.6	3.3	-0.1	7.6	12.4	2.3	3.5	5.2	0.5	3.7	16.1
2.2	7.8	12.6	-0.1	5.5	1.9	1.2	9.1	17.1	1.6	3.9	13.5	0.7	2.8	5.2	2.6	2.7	3.4	0.7	8.6	7.1	0.7	1.3	5.5
1.9	2.2	3.3	2.3	3.5	4.6	0.2	-8.8	1.7	-1.3	-2.2	5.8	-10.9	-11.6	9.2	0.5	1.7	2.8	0.3	3.9	2.4	-2.0	-2.7	2.0
cyclohexanol	AVG		-3.1	-2.7	-1.1	-10.7	9.5	-10.4	-12.6	13.0	-6.7	-4.6	-13.8	-4.2	-1.4	0.3	0.7	4.2	-1.8	-7.1	0.5	0.1	
0.8	-8.2	-5.4	-0.3	-2.4	-4.7	-0.6	0.3	-2.4	-2.3	5.5	7.0	2.3	0.8	1.5	2.9	2.5	12.6	6.7	6.1	9.8	1.2	-4.5	-4.1
1.0	-2.5	3.0	-7.6	-0.1	10.2	1.4	-1.7	6.4	3.8	-0.3	1.2	4.1	-0.7	3.1	2.4	-3.0	2.9	3.6	-0.9	-9.2	3.0	7.9	15.0
-22.2	0.1	10.1	-15.7	0.3	1.9	2.9	2.9	41.2	6.7	21.4	53.9	-10.3	40.5	52.5	-6.1	-0.1	11.3	3.2	-0.1	0.6	-2.6	7.0	11.7
7.4	18.5	19.0	27.1	-0.8	3.0	9.4	7.2	6.0	13.5	4.2	3.7	5.4	1.7	-0.1	0.1								
cyclohexanol	1		-2.2	-4.0	-0.4	-11.7	7.9	-15.1	-16.8	13.0	-8.0	-8.4	-18.3	-6.8	-3.9	-0.4	-0.3	1.7	-4.7	-11.4	-2.0	-2.6	-0.8
-9.1	-7.1	-2.1	-4.0	-4.7	0.5	-0.1	-2.6	-4.0	4.1	6.9	2.1	-0.6	0.3	1.7	1.6	10.1	5.6	3.4	0.7	-1.8	-8.8	-6.0	-1.5
-3.8	3.7	-9.0	-0.2	10.3	0.7	-2.6	7.3	2.1	-5.1	-3.4	2.5	-3.0	-0.8	1.5	-5.0	1.5	3.3	-4.0	-9.6	2.0	6.4	14.1	-21.4
-0.7	10.4	-16.4	-1.8	-0.2	1.7	-1.2	36.9	6.0	18.1	51.4	-9.8	37.1	49.9	-9.2	-0.4	8.1	1.6	-0.9	-0.6	-1.1	3.7	6.9	6.8
11.5	13.7	24.5	-5.0	-5.0	7.7	2.9	2.1	11.4	-0.9	2.9	3.2	-0.3	-1.3	0.9									
cyclohexanol	2		-5.7	-3.8	-4.3	-13.2	7.8	-13.3	-14.4	12.0	-10.5	-5.8	-14.3	-8.5	-2.2	-1.6	0.5	5.7	-3.4	-10.6	0.3	0.3	1.4
-5.7	-3.4	0.9	-1.6	-5.1	-0.8	0.4	-2.4	2.3	3.5	4.0	-0.7	0.2	0.2	2.3	2.8	9.5	6.9	7.1	-1.0	4.0	-1.1	-2.4	5.1
-2.4	3.3	-5.5	0.0	8.3	1.9	-2.3	3.3	1.7	0.9	1.6	2.3	-0.7	2.5	0.2	-2.6	6.4	3.4	0.2	-5.4	2.6	4.8	9.8	-16.6
0.1	8.1	-12.0	-0.1	2.4	1.0	3.3	34.6	4.2	21.0	47.1	-7.7	31.5	39.9	-6.6	-0.3	9.0	2.9	-0.4	0.1	-0.6	9.2	13.2	9.6
15.2	16.1	25.9	2.4	1.9	11.0	6.5	5.8	11.4	10.7	2.7	6.2	2.0	3.9	1.5									
cyclohexanol	3		-6.7	-3.1	-1.6	-12.2	9.6	-10.7	-11.1	14.6	-3.2	-5.4	-6.4	-1.4	-1								

cyclopentanol	AVG	-0.9	-1.3	0.3	-7.2	4.0	-10.0	-14.4	6.8	-8.2	-9.0	-14.9	-9.5	-3.1	-1.0	-1.3	4.6	-4.2	-10.7	-0.1	0.3			
	-0.9	-4.5	-3.8	-0.5	-7.5	-7.9	-3.2	-3.6	-9.8	-6.9	1.6	4.5	1.6	-1.3	-0.9	-1.3	-0.2	12.2	-0.2	-2.0	3.7	-0.1	-2.4	-4.1
	-4.9	-2.7	3.3	-10.1	-0.4	10.0	1.8	-2.1	3.3	-5.8	-3.5	-3.4	-2.9	-0.2	-0.2	2.4	-2.9	5.3	3.8	-0.7	6.2	10.8	-2.6	4.9
	0.5	-3.6	4.6	0.6	-2.8	-1.1	1.9	-1.3	8.0	7.2	-0.8	6.2	3.9	-1.6	5.0	12.6	-0.5	12.3	2.6	0.1	2.2	-4.9	-4.2	-0.3
	4.2	8.0	10.4	21.3	1.1	-1.8	10.0	6.1	8.2	18.4	17.2	-1.9	0.1	0.3	2.4	-4.4								
phenol	1	-1.1	-0.7	3.5	1.3	1.1	-9.3	0.3	7.2	5.8	-1.5	-4.1	1.3	-2.0	-3.2	6.6	-6.6	-5.8	2.1	3.4	-1.4	-4.7	3.7	
	-3.3	1.2	0.4	2.6	1.8	12.1	37.0	-7.9	0.8	2.3	-14.7	1.6	1.3	7.0	-1.8	-21.2	-19.2	-6.7	-7.2	-7.8	-0.7	-16.4	-46.3	-77.8
	-105.3	4.2	-0.9	-32.0	16.7	-2.8	-77.9	-32.5	3.6	-23.1	-42.8	-5.2	-39.7	-13.2	-48.3	-39.3	43.9	-38.9	-92.5	7.1	10.0	3.9	-33.8	
	1.0	-0.4	-25.6	11.2	-5.5	-14.6	2.4	30.5	3.2	2.2	-11.3	-25.8	29.1	12.5	-24.3	-0.7	5.5	-28.0	-9.6	-17.7	-0.5	7.6	5.4	-4.1
	56.9	32.0	14.8	0.3	11.7	-8.2	25.9	55.8	-19.2	-22.3	5.5	0.0	-3.0	-31.2	-1.3									
phenol	2	-4.6	-3.3	-3.2	-4.0	-2.9	-12.2	-5.6	-0.4	0.6	-5.6	-6.6	-5.0	-2.9	-2.7	1.7	-4.8	-5.1	1.9	3.1	-0.6	-6.4	1.8	
	-2.3	1.1	0.6	0.3	1.5	5.6	25.8	-15.9	-3.3	0.0	-17.3	0.1	-1.0	0.7	-0.1	-20.3	-17.2	-1.0	-4.0	-3.1	-0.2	-12.4	-42.8	-75.4
	-100.8	4.2	0.1	-30.9	10.3	-1.9	-75.2	-34.7	2.8	-18.9	-44.9	-0.2	-32.8	-13.4	-39.2	-37.6	43.2	-32.0	-87.1	4.3	8.5	4.4	-30.4	
	2.1	-0.4	-25.8	12.5	-7.2	-19.8	2.0	38.0	0.8	9.2	-6.8	-26.8	29.0	12.5	-24.4	0.4	5.8	-27.7	-7.1	-18.4	-4.0	12.6	12.3	-3.5
	68.0	36.5	16.9	0.7	15.4	-10.3	22.8	52.7	-23.2	-30.4	-1.5	-3.1	-2.8	-34.2	-6.7									
phenol	3	-1.5	-1.7	-1.6	-0.1	-0.1	-11.2	-2.4	3.4	3.5	-3.1	-5.3	-1.3	-3.6	-2.9	1.8	-6.1	-5.2	1.5	1.3	-2.4	-10.4	-0.6	
	-3.2	-1.1	-0.9	-1.4	-2.6	3.1	22.8	-17.2	-5.5	-0.6	-18.2	-1.6	-1.3	0.8	0.0	-21.5	-21.5	-8.4	-7.9	-10.6	-0.5	-17.9	-47.7	-77.2
	-105.1	5.4	0.6	-33.1	13.1	-2.1	-77.6	-34.2	1.8	-22.6	-49.2	-1.1	-35.7	-9.6	-47.9	-44.1	47.2	-42.2	-100.6	5.4	8.9	3.2		
	-37.5	0.8	-1.0	-30.2	12.8	-6.4	-20.4	1.5	40.2	3.8	9.1	-3.0	-33.3	33.8	18.9	-27.0	0.0	5.4	-28.7	-9.9	-19.3	-4.4	9.5	10.1
	-8.7	68.8	39.8	15.7	0.7	12.5	-13.0	21.8	54.7	-23.4	-28.2	0.6	-1.8	-2.5	-35.5	-5.8								
phenol	AVG	-2.4	-1.9	-0.4	-0.9	-0.6	-10.9	-2.6	3.4	3.3	-3.4	-5.3	-1.7	-2.8	-2.9	3.4	-5.9	-5.4	1.8	2.6	-1.5	-7.2		
	1.6	-2.9	0.4	0.1	0.5	0.2	6.9	28.5	-13.6	-2.7	0.6	-16.7	0.0	-0.3	2.8	-0.7	-21.0	-19.3	-5.3	-6.4	-7.2	-0.5	-15.6	-45.6
	-76.8	-103.7	4.6	-0.1	-32.0	13.4	-2.2	-76.9	-33.8	2.7	-21.6	-45.6	-2.2	-36.1	-12.1	-45.1	-40.3	44.8	-37.7	-93.4	5.6	9.2	3.9	
	-33.9	1.3	-0.6	-27.2	12.2	-6.4	-18.2	1.9	36.2	2.1	6.9	-7.0	-28.6	30.6	14.6	-25.3	-0.1	5.6	-28.1	-8.9	-18.5	-3.0	9.9	9.3
cycloheptanol	AVG	-0.8	-1.7	0.5	-7.6	7.7	-12.0	-6.5	13.2	-4.9	-1.4	-14.6	-3.3	-0.3	0.3	-0.8	4.6	-2.7	-8.8	-0.2	-0.7			
	-1.5	-1.2	-0.8	0.2	0.9	0.5	3.6	0.5	-0.6	-2.6	1.0	3.5	-0.7	1.6	-0.1	0.3	9.2	5.7	-1.6	2.8	4.0	0.0	0.5	
	7.5	0.5	5.7	-4.6	-0.3	8.6	-2.0	-0.1	6.6	2.1	-1.2	0.0	5.9	0.0	-1.3	-5.9	-1.0	0.9	1.3	-0.3	12.0	8.6	-1.9	3.4
	-2.3	-3.2	3.8	-1.6	-2.1	-1.8	1.1	-1.1	2.5	0.9	-1.7	5.7	-2.1	-8.1	-2.8	6.0	-0.3	1.7	-1.6	-0.2	2.3	0.6	-3.5	-0.9
cycloheptanol	1	1.3	-0.6	4.3	-7.0	8.9	-9.7	-6.4	14.9	-2.8	-0.4	-12.3	-1.3	0.4	0.3	-0.7	5.7	-2.6	-9.8	0.2	0.4	-1.3		
	0.4	1.7	3.8	2.8	4.0	8.1	1.3	1.7	-0.4	1.6	4.3	-1.3	3.2	1.0	0.8	-0.1	8.8	7.6	-0.8	3.4	5.3	-0.3	1.7	9.7
	1.1	9.8	0.1	-0.8	11.3	0.6	0.4	6.7	2.2	0.4	1.2	4.9	0.0	-0.1	-6.0	2.0	3.2	3.2	0.0	14.2	10.7	0.0	4.9	1.4
	-1.2	6.0	1.0	-0.9	-1.9	4.5	-0.5	2.1	2.1	-0.3	6.5	0.2	-8.1	-4.0	6.7	-0.6	3.8	-0.6	0.7	2.5	-0.1	-3.0	-0.5	4.0
cycloheptanol	2	-2.5	-2.4	-1.8	-8.2	6.1	-15.8	-7.8	13.9	-6.4	-1.5	-14.1	-3.9	-1.2	0.7	-1.0	5.1	-2.7	-10.7	-0.7	-1.4	-3.0		
	-0.4	-0.4	0.8	1.1	0.2	3.7	-1.1	-0.6	-3.1	1.5	2.4	-1.1	1.2	-0.9	-0.8	0.2	9.1	5.2	-1.3	3.5	4.5	-0.1	1.2	8.6
	0.4	4.7	-3.9	-0.3	6.9	-3.4	-0.6	6.4	2.3	-2.1	-0.2	4.8	-0.2	-2.1	-5.7	-1.9	0.6	0.4	-0.2	13.0	8.6	-2.0	2.6	-3.1
	-3.7	3.1	-2.3	-3.0	-2.2	-0.8	-0.9	-0.3	1.1	-2.3	3.8	-2.0	-11.2	-6.5	2.9	-0.3	1.8	-2.7	-0.5	2.4	0.5	-5.7	-2.5	-1.8
cycloheptanol	3	-2.1	-1.9	0.3	-9.2	6.3	-15.1	-7.9	11.8	-7.8	-3.2	-16.1	-4.5	-1.1	-1.3	-0.7	2.1	-3.1	-6.5	-0.5	-1.6	-1.1		
	-1.5	-2.4	-2.5	-1.3	-2.7	-0.6	-0.1	-2.7	-3.6	-0.4	2.5	-0.4	-0.2	-1.2	-0.4	0.1	8.8	3.2	-3.9	0.6	0.9	-0.5	-1.4	3.9
	0.5	2.9	-4.9	-0.3	5.9	-4.2	-0.9	4.7	-0.3	-4.8	-2.8	6.8	0.4	-3.7	-5.4	-2.7	-1.9	0.1	-0.5	9.3	7.6	-3.7	2.2	-4.8
	-5.0	1.7	-5.3	-3.8	-3.3	-1.2	-3.8	2.7	-1.0	-4.6	4.7	-4.6	-7.3	-1.6	6.1	0.2	-0.1	-2.1	-1.0	1.8	0.3	-3.7	-0.8	0.9
2-hexanol	AVG	-0.4	-1.5	0.5	-5.4	9.9	-9.9	-10.4	9.3	-10.3	-6.0	9.5	-3.2	-1.0	0.8	1.2	6.1	0.0	-6.1	2.5	1.8	1.7		
	-2.6	-2.6	2.2	5.0	-4.8	0.6	0.1	1.6	4.0	1.2	5.1	1.6	1.9	0.6	1.7	-0.1	18.5	10.1	2.1	13.9	5.4	-1.3	1.4	8.3
	-0.8	5.2	-3.6	0.2	13.9	5.4	-0.8	7.5	11.2	-0.5	1.5	15.4	0.0	7.0	16.6	-1.6	5.1	6.9	-0.2	8.5	20.6	7.7	10.4	1.0
	7.4	8.2	1.9	7.1	11.5	12.7	-0.6	8.4	6.3	4.1	15.1	9.4	15.7	24.1	26.0	0.4	12.7	11.5	-0.3	9.9	-0.1	-3.4	3.1	7.2
	18.2	18.8	23.4	1.0	-2.0	14.5	12.7	11.2	13.8	4.7	5.5	1.5	0.0	-2.1	-4.5									
2-hexanol	1	-0.9	-1.7	2.0	-8.7	8.8	-10.5	-12.3	9.2	-9.4	-5.6	10.9	-3.1	-1.6	0.9	-0.2	5.4	-0.6	-7.2	3.4	1.5	3.5		
	-3.7	-0.9	5.3	-4.9	3.7	-1.2	-1.7	2.4	0.4	3.5	0.2	0.7	-0.7	0.6	-0.5	21.4	13.7	4.3	18.3	11.9	-0.4	0.5	13.2	
	-1.6	6.6	-8.7	0.5	15.0	4.9	-1.1	9.0	10.6	0.3	3.2	18.0	0.2	9.1	19.2	-0.7	6.6	10.5	-0.2	9.6	23.3	8.1	12.4	1.1
	9.1	10.9	0.8	9.6	12.8	17.8	2.0	12.2	7.6	6.0	19.5	12.9	17.8	25.5	28.4	0.7	16.7	11.9	-0.2	13.4	0.4	-0.2	5.2	8.7
	18.6	19.5	25.7	1.8	-1.9	16.3	13.9	12.8	15.5	4.2	7.9	0.4	0.7	-2.4	-7.1									
2-hexanol	2	-1.4	-2.5	-0.3	-7.2	8.7	-13.0	-8.7	9.3	-10.0	-3.2	8.6	-2.9	-0.3	1.1	1.4	6.4	-1.0	-9.2	0.6	-0.2	-0.8		
	-3.1	-4.6	-0.5	-5.4	-3.9	-1.5	1.9	-0.8	7.9	1.5	5.8	1.4	2.7	0.4	0.4	0.1	14.0	8.4	-1.0	10.2	1.0	-2.6	-2.2	5.6
	-0.2	4.8	3.5	-0.4	10.9	2.7	-2.0	6.6	9.8	-2.5	-0.5	15.2	0.0	6.8	16.5	-1.3	4.6	5.6	-0.3	9.3	16.6	3.5	6.5	-0.3
	3.4	5.6	2.3	7.6	14.4	12.5	-0.3	7.2	6.4	3.5	10.2	9.1	13.9	21.2	27.3	0.2	9.0	9.6	-0.5	8.7	1.6	-0.6	5.8	9.9
	19.3	19.7	23.5	1.6	-0.7	13.1	10.5	11.0	12.1	4.6	5.2	2.4	-0.3	-2.4	-6.2									
2-hexanol	3	1.0	-1.0	1.2	-3.3	11.8	-8.4	-10.9	7.0	-12.2	-6.7													

3-hexanol	3	-4.3	-3.6	-1.0	-5.4	6.7	-3.3	-11.8	6.9	-7.4	-6.8	9.8	-2.0	0.4	1.1	1.8	14.0	-1.5	-9.2	4.5	4.7	5.0		
	-4.8	-3.0	2.2	-8.5	-8.5	-1.4	-0.4	-1.8	1.2	0.0	2.7	-1.6	-2.3	-3.2	-1.6	-0.1	16.0	6.8	0.3	11.5	3.5	-3.5	-3.4	11.1
	-4.0	2.9	5.9	0.0	7.9	2.1	-6.9	2.4	6.4	0.0	5.3	20.5	0.4	9.4	16.6	-4.3	2.9	5.1	-2.9	1.7	12.7	2.7	5.0	-7.3
	3.6	4.0	-4.5	6.9	10.2	10.4	1.2	8.6	3.1	4.6	17.2	4.5	18.8	28.7	21.0	0.3	8.6	7.0	0.7	6.5	-1.7	-9.3	-1.6	4.0
	17.2	23.4	19.3	-0.7	-4.5	10.0	2.8	10.4	23.7	7.6	5.8	5.0	0.4	-2.5	-6.2									
3-hexanol	2	-3.3	-2.9	-0.5	-4.0	11.0	-2.0	-10.7	15.4	-5.4	-7.2	12.3	-1.6	2.0	2.6	2.2	8.7	3.3	-0.2	5.2	4.4	6.5		
	-3.2	-3.8	3.0	-4.2	-6.1	3.8	-0.4	-1.1	1.9	2.8	5.4	3.3	0.9	2.7	4.6	-0.3	17.3	9.9	0.9	13.3	5.9	-1.7	-1.9	12.4
	-1.9	6.6	2.1	-0.3	15.2	3.5	-2.3	8.9	11.1	-1.6	0.8	21.3	0.3	11.4	22.5	-3.4	3.4	4.8	-0.4	2.0	17.0	8.5	11.2	-5.6
	9.9	10.1	-1.6	8.4	11.7	14.0	0.6	11.4	2.6	9.0	27.7	6.7	26.5	36.9	22.1	0.2	15.6	10.0	-0.2	7.2	-4.5	-2.5	5.3	9.6
	21.2	25.7	26.9	1.0	-2.8	14.8	9.3	15.0	19.1	3.3	6.6	3.0	-0.2	-1.9	-3.4									
cyclohexanol	AVG	-1.9	-1.2	0.0	-7.4	6.8	-11.5	-9.9	7.5	-5.8	-5.1	-24.9	-7.5	-1.3	0.2	0.2	7.2	-2.8	-8.2	-0.6	-1.0			
	-1.5	-5.3	-5.1	-3.0	-4.3	-4.7	-0.6	1.1	-0.6	-3.4	0.9	3.5	0.0	2.3	0.3	0.5	-0.2	12.6	1.4	-2.3	3.4	-0.5	-0.7	-3.2
	-2.0	0.0	4.6	-9.0	-0.1	11.7	3.4	-0.5	5.7	0.2	-2.0	-2.0	0.1	-0.3	-1.0	2.6	-1.8	3.1	2.7	0.0	-8.5	2.3	7.5	11.8
	-18.7	-1.2	6.6	-11.6	5.0	9.4	8.5	3.1	45.1	7.1	24.4	58.1	-14.1	50.8	67.7	5.2	0.4	9.9	-2.3	-0.3	-0.2	-2.7	7.8	11.3
cyclohexanol	2	-1.5	-2.1	-1.5	-7.2	7.9	-10.9	-6.0	10.5	-1.5	-1.1	-27.6	-6.4	-0.2	0.7	0.7	7.6	-2.8	-8.9	-0.4	-1.1	-1.2		
	-2.2	-2.7	-1.5	-1.4	-1.1	2.3	2.0	-1.0	-2.3	-0.1	2.9	-0.5	2.0	-0.3	-0.2	-0.3	9.8	0.0	-1.5	1.3	2.7	-0.5	-0.2	0.0
	0.6	3.2	-11.8	-0.4	9.9	1.2	-0.4	4.7	-0.3	-1.1	-2.4	-1.1	-0.7	-1.9	-0.8	-1.8	0.7	1.6	0.0	-7.6	0.1	5.1	8.4	-16.0
	-3.0	4.4	-9.1	4.0	7.0	6.3	1.9	38.9	3.6	21.4	51.3	-12.8	45.1	59.4	3.3	0.3	8.3	-2.8	-0.8	-0.9	-0.6	5.2	8.7	3.4
cyclohexanol	3	-2.7	-2.2	-0.6	-8.3	5.0	-15.2	-11.6	6.1	-7.2	-5.5	-24.1	-7.2	-2.0	-0.6	-2.0	5.7	-2.6	-8.3	-0.8	-0.8	-1.4		
	-5.8	-5.6	-3.1	-5.8	-6.3	-2.3	-0.3	-0.9	-6.4	0.6	2.4	-0.9	2.9	0.4	0.5	-0.3	13.4	1.9	-2.7	3.6	-2.4	-1.1	-5.2	-4.6
	-0.2	3.3	-15.7	0.1	12.4	5.1	-0.4	5.9	-0.5	-0.9	-1.4	0.5	-0.3	-0.1	5.6	-2.0	4.7	3.1	0.0	-8.7	0.1	9.3	12.9	-18.9
	0.7	8.4	-12.7	5.9	10.5	8.9	5.3	51.9	9.7	30.0	67.2	-14.0	53.8	69.7	1.8	0.5	10.6	-3.1	0.0	-0.1	-2.6	10.5	13.9	6.1
cyclohexanol	1	-1.6	0.6	2.1	-6.8	7.4	-8.5	-12.0	5.9	-8.6	-8.6	-23.0	-8.7	-1.7	0.4	2.0	8.3	-3.0	-7.4	-0.6	-1.1	-1.8		
	-7.8	-6.9	-4.4	-5.6	-6.8	-1.8	1.6	-0.1	-1.4	2.0	5.4	1.3	2.0	0.8	1.3	-0.1	14.5	2.4	-2.6	5.2	-1.6	-0.7	-4.2	-1.3
	-0.3	7.3	0.6	0.0	12.7	3.8	-0.8	6.4	1.3	-4.0	-2.1	0.9	0.1	-0.9	2.9	-1.7	3.9	3.4	0.0	-9.1	6.6	8.2	14.1	-21.2
	18.4	21.5	21.4	-0.7	-3.1	6.0	-0.9	-0.2	17.2	-0.6	-2.1	-3.3	-0.7	-9.4	-12.9									
hexanol	1	-2.8	-3.4	-1.8	-6.7	8.2	-13.0	-8.1	9.2	-7.2	-1.9	-12.3	-4.2	1.0	1.7	0.2	2.6	1.0	-3.4	2.5	3.4	0.0	-1.1	
	-3.0	2.2	-0.7	-1.1	3.5	4.3	0.8	5.6	4.2	7.1	2.4	1.3	0.8	-0.8	-0.6	13.0	5.7	1.2	8.0	3.6	-1.0	0.1	7.6	-0.1
	6.1	-1.4	0.1	14.7	5.2	-0.9	8.0	13.6	-0.9	0.6	11.3	-0.1	3.9	17.5	-5.4	1.3	1.7	0.2	2.3	10.7	3.6	4.4	-0.5	3.1
	3.1	2.1	9.3	13.3	12.2	-1.6	9.3	3.3	1.2	5.4	3.7	15.4	21.9	20.9	-0.3	5.0	2.3	-0.3	5.6	1.2	1.0	3.0	5.7	22.6
hexanol	2	-1.2	-2.3	-1.7	-8.0	8.9	-11.4	-5.7	11.0	-5.8	-2.4	-11.2	-3.4	-1.8	1.1	-0.5	3.0	-1.1	-6.9	2.3	2.6	1.3	-1.2	
	-3.6	0.2	-2.7	-4.0	0.0	0.7	-0.2	1.6	2.4	5.2	1.6	0.5	-0.4	-1.1	-0.5	13.0	6.2	1.7	11.1	3.7	-0.1	-1.0	6.4	-0.9
	2.6	-7.5	-0.3	12.0	3.9	-1.1	5.6	9.0	-0.8	1.8	14.9	0.1	4.6	14.8	-1.9	2.0	3.7	-0.3	2.6	13.4	3.7	5.8	-1.6	3.3
	4.4	-1.7	13.4	18.3	14.7	0.8	10.1	7.0	2.2	10.8	6.7	19.5	28.5	24.7	0.0	8.4	6.4	-0.6	3.8	-3.7	-2.4	2.7	5.6	23.3
hexanol	3	-2.6	-2.4	-1.1	-5.7	10.0	-5.3	-9.4	10.4	-9.8	-2.4	-8.9	0.5	-0.6	1.7	1.6	3.0	-0.7	-2.4	2.0	2.2	1.0	-4.1	
	-3.9	0.1	-4.3	-4.2	3.5	2.5	0.9	3.3	2.4	4.8	2.2	-2.3	-1.0	0.4	0.4	14.8	8.6	1.2	12.7	5.1	-1.3	-1.2	9.8	-0.4
	4.1	-9.8	0.0	17.1	7.3	-2.7	7.7	15.6	-2.0	0.1	16.3	-0.3	6.5	13.0	-1.2	2.6	6.6	-0.4	5.0	17.7	8.9	12.6	1.5	8.5
	10.4	4.6	8.6	12.9	15.4	0.0	15.3	10.1	2.2	14.7	9.2	20.6	30.3	23.8	-0.1	14.4	10.8	0.3	10.4	1.4	-0.9	1.6	5.3	19.7
hexanol	4	-3.4	-3.2	-1.0	-6.5	7.8	-12.5	-10.6	10.9	-10.1	-6.1	-6.4	-4.1	-1.6	-0.2	-0.2	1.4	0.8	-2.1	2.8	1.9	0.7	-3.7	
	-2.1	1.7	-3.0	-1.9	2.1	2.8	0.4	4.2	3.0	6.4	2.8	0.0	1.3	1.9	-0.3	18.1	15.8	3.2	13.6	11.1	0.0	3.0	18.1	0.1
	9.6	6.5	0.1	19.0	5.3	-0.3	9.6	17.3	-2.4	0.6	19.4	-0.1	8.4	17.5	1.6	6.0	8.3	0.1	13.7	22.9	11.0	14.9	4.3	10.0
	13.5	4.6	8.1	12.4	16.4	1.3	12.9	11.7	3.8	11.5	11.6	17.6	28.7	32.3	0.4	16.4	11.8	0.1	10.7	0.9	1.6	4.0	10.0	23.3
hexanol	5	-4.4	-4.9	-2.3	-7.6	8.5	-10.5	-14.0	8.8	-15.8	-7.6	-2.9	-1.6	-1.6	-0.1	3.0	3.9	0.7	-1.3	2.8	2.6	0.1	-5.4	
	-4.4	-0.6	-4.4	0.0	2.2	-0.4	3.1	5.7	7.9	6.6	3.1	2.7	3.5	1.0	15.9	9.0	1.9	14.1	7.0	-0.9	-0.1	15.2	0.3	
	7.8	2.6	1.0	19.6	2.2	0.3	12.2	19.2	-3.4	2.3	23.5	-0.2	10.0	17.9	-0.8	4.6	6.9	-0.3	11.8	21.5	9.4	13.0	1.2	9.2
	10.1	2.1	10.4	14.1	19.3	3.4	17.8	16.5	6.6	15.5	11.8	18.0	30.7	29.6	0.6	13.7	11.2	-0.1	9.1	-2.4	5.8	8.6	8.9	31.4
hexanol	AVG	-2.2	-2.5	-1.4	-6.7	8.9	-9.9	-8.7	10.4	-9.3	-3.4	-7.7	-2.5	-0.6	0.9	1.1	2.7	-0.6	-4.3	2.4	2.4	0.8		
	-2.1	-2.9	0.9	-1.9	-2.1	2.2	2.2	0.6	4.2	3.6	6.1	3.2	1.1	1.0	1.1	-0.1	13.9	9.4	1.9	10.5	5.8	-0.4	0.8	11.9
	0.3	6.4	0.5	0.2	14.5	4.4	-0.4	8.4	14.9	-1.1	1.6	15.5	0.0	6.1	14.1	-0.6	3.3	5.0	0.0	7.4	15.6	6.4	8.8	1.9
	6.0	7.2	2.6	9.0	12.6	13.7	0.8	9.6	8.4	2.6	9.5	8.0	13.3	21.4	23.4	0.3	9.9	7.6	0.3	7.2	0.0	1.0	3.0	5.9
pentanol	AVG	-5.2	-4.6	-2.4	-7.0	9.4	-11.6	-12.6	12.4	-10.1	-5.8	-10.1	-5.9	0.0	1.3	1.2	3.0	1.5	-2.5	3.3	3.0	2.2		
	-4.5	-5.3	1.3	-4.2	-3.8	2.0	1.4	0.3	1.6	5.4	1.0	0.6	1.7	1.3	0.1	16.9	10.7	2.6	13.8	7.2	-3.2	-1.1	11.2	
	-2.0	4.8	-4.2	0.1	16.8	5.1	-1.1	8.4	12.2	1.1	4.1	19.0	0.2	8.1	19.6	-1.6	5.7	7.1	-0.5	7.4	21.9	11.1	14.1	0.4
	11.5	12.9	2.2	13.4	18.8	21.5	3.5	23.9	16.7	7.0	21.1	13.0	26.1	37.2	29.9	0.5	17.7	11.4	0.7	9.7	-1.6	4.9	7.6	7.7
pentanol	1	-6.3	-5.1	-0.7	-8.2	9.1	-13.4	-14.1	11.5	-10.8	-7.2	-7.0	-4.5	0.5	1.5									

2.8	-3.9	-0.2	15.4	1.5	-4.0	5.2	9.7	1.6	3.5	18.4	0.1	7.4	18.5	-3.0	4.0	5.9	-1.0	4.7	20.0	10.9	14.0	-4.0	12.8	
15.4	-1.3	10.6	15.5	19.5	2.4	27.2	18.5	6.3	20.5	10.1	26.9	37.2	27.3	0.6	19.4	11.6	0.5	9.8	-2.9	3.4	6.0	7.2	28.9	
19.5	34.2	0.8	1.6	9.2	17.7	13.4	15.0	3.6	5.3	4.2	-0.1	-4.7	-7.8	-3.3	-0.3	1.0	1.8	0.8	6.1	1.0	-3.4	3.7	3.5	2.9
2-octanol	AVG	-0.2	-1.4	0.8	-4.6	10.8	-10.8	-5.0	5.0	-7.9	-0.9	-3.3	-0.3	1.0	1.8	0.8	6.1	1.0	-3.4	3.7	3.5	2.9		
-4.8	-1.7	2.9	-1.2	-1.8	2.2	1.7	0.9	3.3	1.3	4.6	3.7	4.1	2.6	2.8	0.3	13.8	17.9	1.0	8.0	5.8	-1.6	0.5	17.3	
0.3	9.4	12.5	-0.1	13.5	4.9	0.6	14.8	29.2	0.1	4.0	15.7	0.1	11.2	19.1	0.7	3.3	3.8	0.2	2.6	12.2	3.9	5.4	-3.0	
4.0	5.5	-2.4	15.6	23.2	20.9	3.2	20.3	3.2	11.5	23.8	-0.6	34.1	49.0	22.1	0.4	4.8	3.2	0.5	5.4	0.8	1.6	6.5	5.4	
23.5	24.2	24.0	-0.7	-3.9	7.0	9.5	1.1	6.7	0.8	2.6	0.6	0.5	-5.0	-7.7										
2-octanol	1	0.2	-0.2	2.0	-3.7	8.6	-10.5	-6.9	2.6	-7.7	-3.7	-5.5	-2.0	0.3	2.4	2.1	7.3	4.4	-0.7	2.4	2.7	4.5		
-6.7	-3.1	1.5	-7.1	-7.3	-1.3	2.7	1.6	3.8	0.5	4.3	2.7	4.9	1.9	4.2	0.3	17.5	21.6	0.2	10.2	7.2	-4.3	-2.0	17.3	
-0.4	9.2	7.0	0.0	16.5	8.4	1.2	18.5	31.8	2.5	4.4	16.6	0.1	12.5	20.8	1.5	4.7	7.4	0.0	6.1	17.9	8.4	9.9	3.5	
5.5	7.7	-1.3	16.3	23.9	21.5	5.9	25.9	7.2	19.4	33.9	4.9	41.0	56.1	27.2	0.5	10.3	4.4	1.6	8.8	-0.2	4.0	9.6	6.5	
26.2	28.5	29.2	4.0	0.9	13.8	11.8	3.1	10.7	0.2	5.3	3.3	2.4	-4.9	-9.6										
2-octanol	2	-0.2	-2.0	0.9	-5.3	10.4	-11.7	-3.9	6.7	-7.8	0.9	-1.8	-0.5	1.1	1.8	-0.1	5.6	0.3	-4.0	5.4	4.5	2.3		
0.0	-0.5	4.3	2.6	2.6	4.4	2.8	1.7	6.3	2.3	5.6	4.0	5.5	4.8	4.4	0.2	11.9	16.1	2.2	6.4	5.8	-0.5	2.0	15.8	
0.9	8.6	14.3	-0.3	12.5	3.4	0.5	15.2	27.7	-0.8	3.2	13.8	0.1	9.3	16.5	0.0	2.3	0.9	0.1	1.2	9.6	1.2	2.6	-5.8	
2.2	2.7	-2.3	14.2	19.5	18.8	1.8	14.7	0.1	7.0	17.6	-2.4	31.5	44.5	19.9	0.5	2.0	2.5	0.1	3.6	2.6	0.2	4.0	3.6	
19.7	19.7	20.1	-2.6	-4.8	2.7	10.4	0.7	4.7	2.8	2.0	-0.2	0.4	-4.2	-5.5										
2-octanol	3	-0.6	-1.9	-0.6	-4.8	13.3	-10.2	-4.3	5.7	-8.1	0.1	-2.7	1.7	1.6	1.4	0.4	5.3	-1.7	-5.6	3.2	3.3	2.1		
-7.5	-1.5	2.9	0.9	-0.7	3.6	-0.2	-0.7	-0.1	1.0	3.9	4.4	1.8	1.2	0.0	0.2	12.1	15.9	0.6	7.4	4.6	0.1	1.6	18.9	
0.4	10.3	16.3	0.0	11.4	2.8	0.2	10.7	27.9	-1.5	4.3	16.6	0.0	11.6	20.0	0.6	3.0	3.3	0.3	0.4	9.1	2.0	3.7	-6.7	
4.5	6.0	-3.6	16.3	26.1	22.4	2.0	20.2	2.3	8.1	19.9	-4.2	29.8	46.5	19.3	0.3	2.0	2.8	-0.2	4.0	-0.1	0.6	5.8	6.2	
24.6	24.5	22.8	-3.4	-7.7	4.6	6.2	-0.6	4.8	-0.5	0.5	-1.3	-1.4	-5.8	-8.1										
octanol	AVG	-0.1	-1.4	0.0	-6.5	9.8	-12.2	-6.4	5.8	-9.0	-1.6	-5.9	-2.3	-0.5	1.0	0.3	3.7	-0.7	-5.1	0.2	-0.4	-0.6		
-2.3	-4.5	-0.5	-1.9	-2.0	-0.4	0.7	-0.2	1.1	-1.7	1.5	0.8	0.9	-0.5	-0.2	-0.1	9.7	8.9	0.2	5.3	4.1	-0.2	-0.2	8.5	
0.1	6.8	8.4	-0.2	7.5	3.2	-0.2	4.3	12.1	-2.1	0.2	8.7	-0.1	6.4	15.6	-0.3	0.7	1.7	-0.2	3.6	10.5	1.0	2.8	-1.5	
0.1	1.2	-2.1	14.3	22.6	20.4	0.0	6.0	2.8	1.5	8.6	3.0	21.2	32.9	30.0	0.3	0.3	4.5	-0.4	5.2	2.3	0.8	2.5	5.1	
octanol	2	0.8	-0.6	0.6	-5.4	9.8	-12.7	-4.8	6.6	-8.0	-1.1	-7.5	-1.3	-0.1	1.4	1.2	3.9	0.2	-3.5	-0.7	-0.9	-2.5	-1.3	
-2.5	0.3	-0.1	-0.4	1.2	-0.5	-0.9	1.0	-1.4	1.8	-0.3	1.3	0.5	-0.3	-0.2	12.4	10.9	1.4	5.9	5.2	0.5	-0.5	7.0	0.9	
6.4	7.0	-0.3	7.2	4.6	0.4	4.4	10.4	-1.4	0.5	6.2	-0.5	6.2	14.1	-0.6	0.5	1.9	-0.2	5.3	11.7	2.0	2.1	-0.4	1.1	
2.8	0.3	14.7	21.6	19.5	-1.5	3.4	3.1	-0.1	6.0	3.8	20.0	30.5	32.1	0.0	1.8	6.5	-0.3	7.4	4.5	-1.3	-1.6	2.1	21.0	
octanol	3	-1.9	-3.1	0.2	-9.4	7.5	-16.0	-8.3	3.6	-11.4	-3.4	-7.3	-4.6	-0.6	-0.4	-0.9	2.9	-2.4	-7.5	-0.2	-1.7	0.4	-4.8	
-7.6	-3.3	-4.2	-4.7	-3.6	2.4	-0.3	1.5	-1.5	1.2	-0.7	0.3	-1.6	-0.1	-0.9	8.6	6.7	-0.2	5.5	1.8	-0.3	0.9	7.6	-0.8	
7.3	9.6	0.1	6.5	2.9	-0.9	2.3	9.6	-1.9	0.6	10.7	0.1	7.8	19.4	0.7	1.6	2.8	-0.1	4.3	9.2	0.8	3.4	-1.3	-0.2	
0.9	-3.4	15.0	23.6	20.7	2.0	6.6	4.6	3.0	10.1	4.6	23.1	34.3	29.5	0.8	0.6	2.0	-0.4	3.4	2.8	0.8	2.9	6.8	23.4	
17.5	27.8	-1.7	-6.2	2.7	13.8	2.0	2.3	0.8	-3.2	-4.0	-1.2	-1.6	-0.7											
octanol	1	0.8	-0.5	-0.8	-4.7	12.0	-8.1	-5.9	7.1	-7.6	-0.4	-2.9	-0.9	-0.9	1.9	0.7	4.2	0.2	-4.1	1.5	1.2	0.2	-0.9	
-3.4	1.4	-1.4	-0.9	1.1	0.3	0.7	0.7	-2.2	1.5	3.3	1.2	-0.3	-0.1	0.6	8.1	9.1	-0.5	4.6	5.3	-0.8	0.7	10.8	0.0	
6.5	8.7	-0.5	8.8	2.1	0.0	6.2	16.2	-3.0	-0.3	9.3	0.2	5.3	13.3	-1.1	-0.1	0.3	-0.2	1.2	10.6	0.3	3.0	-2.9	-0.6	
-0.1	-3.2	13.1	22.5	20.9	-0.5	8.2	0.8	1.7	9.6	0.5	20.4	33.9	28.3	0.0	-1.4	4.9	-0.5	4.8	-0.4	2.8	6.2	6.5	27.9	
21.2	32.0	0.4	-6.2	6.1	13.5	5.1	5.9	3.7	2.1	2.2	0.3	3.6	5.5											
benzene_1	0.4	0.5	1.2	-0.3	0.9	1.6	7.1	-15.9	9.5	3.7	0.3	-2.1	1.0	0.2	0.6	3.2	1.5	0.3	2.4	-0.5	-0.9	0.3		
0.4	1.2	2.4	-0.2	1.3	0.2	1.3	0.0	1.3	1.3	-0.1	0.5	0.0	1.4	0.0	1.3	1.9	2.0	0.7	-0.6	0.9	1.0	2.3	3.2	
1.5	3.9	0.0	1.2	3.6	2.9	3.9	4.0	1.5	2.3	2.7	0.5	2.5	0.5	1.5	1.0	1.6	1.5	1.8	-0.3	1.5	1.3	0.2	1.4	
2.1	1.6	3.5	-0.8	2.1	0.8	0.2	1.2	1.0	2.6	-0.7	-3.0	-2.0	0.9	0.7	1.3	-1.6	0.4	-1.0	-0.1	-0.3	-0.3	-2.0	-0.5	
0.8	1.1	-0.2	-1.7	-0.9	-3.1	-1.3	-0.6	5.0	-1.6	-2.2	2.3	-1.6	-1.6											
benzene_2	-5.7	-5.1	-4.0	-4.5	-11.9	2.3	2.7	-22.5	2.0	1.1	8.8	5.3	3.6	4.0	7.2	4.9	5.4	5.3	-1.1	-2.9	-1.2	-4.7		
-4.4	1.0	-5.0	-7.8	-3.7	3.9	1.1	3.8	2.1	-0.1	4.2	7.7	5.7	8.2	-0.8	-4.3	-0.7	3.7	1.1	1.4	-0.6	-1.2	0.0	2.8	
1.2	-0.3	1.8	4.3	8.0	3.8	4.0	3.2	-0.7	-0.2	-7.3	0.0	-0.1	-2.1	2.4	6.0	4.0	1.2	2.2	3.3	5.3	4.0	9.7	1.6	
0.0	7.5	3.2	0.2	1.8	6.6	1.2	4.8	7.7	5.6	9.0	-1.2	-3.4	4.5	0.2	4.7	6.1	-0.8	0.0	2.1	2.5	2.3	3.7	-1.3	
-0.8	2.0	5.1	5.8	8.6	8.6	1.6	3.5	8.0	6.0	6.4	8.9	2.6	2.4	4.7										
benzene_3	2.1	0.1	2.0	1.3	-1.0	2.9	12.2	-20.5	14.5	4.1	3.6	1.9	-0.4	3.0	3.2	4.3	8.0	2.1	1.6	0.2	0.6	-0.6		
-0.6	1.5	-0.2	0.0	1.0	-1.8	0.4	0.0	2.7	0.3	2.3	1.9	-1.2	1.5	-0.5	1.7	2.5	0.3	1.7	2.0	0.4	-1.7	0.2	0.1	
-0.9	-1.2	1.1	-1.8	1.7	0.3	0.8	5.3	0.0	1.4	0.8	1.3	1.5	1.2	0.4	1.3	4.3	-1.3	-1.2	0.2	1.6	1.0	2.5		
2.2	-1.2	-0.3	0.0	0.2	0.0	2.0	1.9	3.0	3.1	2.5	0.1	1.0	0.2	0.6	1.3	2.0	0.5	1.0	1.1	0.9	1.4	2.4		
3.7	5.8	2.1	3.6	2.5	3.0	1.8	2.8	4.2	2.3	1.1	2.3	1.4	0.0											
toluene_1	-6.6	-5.1	-8.5	3.3	-10.0	4.6	-1.2	-19.0	1.3	-2.8	1.1	1.6	-1.7	4.1	1.7	-1.7	5.8	3.3						

1.8	4.2	2.8	1.2	2.6	4.2	1.2	5.8	4.3	4.4	8.1	4.7	4.4	5.3	3.7	1.7	4.7	4.7	2.2	3.4	0.1	6.9	8.8	8.0	
18.5	17.1	16.3	2.1	2.3	8.9	6.0	5.9	9.7	1.8	6.0	8.1	3.3	5.6	6.8										
paraxylene_1	-2.3	-0.9	0.4	11.4	-11.3	6.3	1.4	-4.2	-2.4	4.2	1.0	3.7	-1.6	3.5	-1.1	0.8	4.1	3.8	3.3	2.8	7.1			
1.9	4.9	5.4	4.2	0.9	6.0	0.4	1.2	0.4	2.7	-0.7	-0.3	0.3	-0.3	3.0	0.3	5.8	5.2	0.9	3.3	2.7	0.4	-1.4	2.2	
-3.0	-0.2	7.5	-1.7	-1.2	0.3	-1.6	0.9	-3.3	-1.3	0.1	2.1	-3.4	-1.4	2.2	-2.2	0.6	-0.6	-3.8	-1.7	1.8	0.9	1.0	-5.6	
1.6	1.4	-4.4	-1.3	-0.4	-0.7	0.4	0.9	-0.2	3.0	11.5	0.3	5.4	6.3	1.1	0.4	0.9	-1.7	-0.3	3.5	4.7	2.8	3.3	4.5	
14.5	11.4	15.8	3.4	5.1	7.8	5.0	6.7	10.6	7.4	8.0	4.1	4.4	5.6	3.1										
paraxylene_2	-4.1	-1.0	-1.6	7.1	-11.4	6.9	-1.7	-1.8	-1.9	0.2	1.9	-1.1	-1.9	2.6	0.3	0.4	3.8	5.2	2.3	1.8	12.6			
-2.2	-2.2	3.1	-0.3	-0.6	4.2	1.7	-0.8	-4.7	0.1	0.1	1.5	0.4	-0.8	1.8	0.4	5.1	6.8	1.4	1.2	2.7	0.6	1.3	6.3	
-0.1	2.6	4.5	-0.4	1.5	2.4	-2.1	2.1	-0.3	3.9	3.7	7.5	-0.6	4.6	5.5	2.5	4.1	4.6	0.6	9.2	2.7	0.1	1.7	2.4	
0.8	0.6	1.1	-0.1	1.4	2.1	-0.5	-6.9	2.9	-1.4	-1.8	4.9	-8.8	-8.8	5.8	-0.7	3.9	0.2	-0.5	2.8	0.0	-3.1	0.9		
8.0	7.5	8.7	-1.0	0.4	2.3	1.5	1.7	5.9	6.2	5.1	3.3	1.0	3.3	1.4										
paraxylene_3	0.6	0.0	0.5	8.7	-9.2	6.0	1.8	-7.1	-3.3	1.5	1.8	1.2	-1.7	3.5	-0.4	0.1	4.3	6.2	5.8	4.1	21.6			
-1.8	-2.9	0.9	0.5	-5.5	13.0	2.1	-0.5	-9.2	3.1	1.8	-0.8	-2.2	-0.8	0.4	-4.2	4.2	-3.8	-1.4	0.9	-1.3	-1.6	-4.9	-1.8	
-1.5	0.5	-0.9	1.3	-2.1	3.0	-0.9	-0.1	-3.9	-2.7	3.2	1.1	-0.4	0.2	-0.2	-0.4	2.5	5.0	-0.2	2.9	1.0	0.5	1.4	-2.2	
4.2	0.9	5.4	-0.8	0.9	0.1	-2.3	-0.9	3.6	1.5	0.6	2.6	-1.9	-0.7	1.6	1.2	0.2	3.5	1.1	4.8	-1.0	-1.3	3.3	0.9	
16.8	16.4	17.9	-1.0	-2.9	-0.2	3.8	1.7	4.9	8.8	5.7	1.8	4.6	3.6	4.4										
paraxylene_Avg	-1.9	-0.7	-0.2	9.0	-10.6	6.4	0.5	-4.3	-2.5	1.9	1.5	1.3	-1.7	3.2	-0.4	0.4	4.1	5.1	3.8	2.9	13.7			
-0.7	0.0	3.1	1.4	-1.7	7.7	1.4	0.0	-4.5	2.0	0.4	0.1	-0.5	-0.6	1.7	-1.2	5.1	2.7	0.3	1.8	1.4	-0.2	-1.6	2.2	
-1.5	1.0	3.7	-0.3	-0.6	1.9	-1.5	1.0	-2.5	0.0	0.2	3.6	-1.4	1.1	2.5	0.0	2.4	3.0	-1.2	3.5	1.8	0.5	1.4	-1.8	
2.2	1.0	0.7	-0.7	0.6	0.5	-0.8	-2.3	2.1	1.1	3.4	2.6	-1.7	-1.1	2.8	0.3	1.6	0.7	0.1	3.7	1.3	-0.5	1.1	2.1	
13.1	11.8	14.1	0.5	0.9	3.3	3.4	3.4	7.1	7.5	6.2	3.1	3.3	4.2	3.0										
tri-n-butylphosphine AVG	0.4	-15.6	2.3	-44.4	28.9	-9.5	-41.9	13.2	-40.5	-13.7	19.5	-27.1	-26.8	1.6	-9.7	24.1	15.9	19.5	2.6					
2.3	-4.3	-39.0	8.3	-14.2	-10.6	-2.2	4.9	4.7	-6.2	5.1	61.0	-20.5	14.2	-3.3	-1.5	-3.8	-0.5	130.1	-67.5	46.9	126.7	-66.1	-42.3	
-18.7	59.1	0.2	26.5	-4.8	-82.5	-14.6	94.7	-15.1	7.8	-7.1	-82.5	-40.5	76.3	-52.7	-25.6	9.7	4.8	46.1	39.1	-1.7	1.4	5.5	1.3	
2.4	1.0	1.8	2.5	1.7	3.4	4.2	4.6	1.9	1.7	5.2	2.4	3.4	6.1	-0.6	0.1	7.8	1.9	-10.7	9.2	2.0	4.4	2.6	0.2	
0.2	6.7	13.1	12.8	15.2	3.8	5.1	7.2	5.9	7.7	10.0	34.6	0.9	2.1	3.2	16.8	6.1								
tri-n-butylphosphine 1	4.1	-13.8	8.0	-40.9	31.2	-6.6	-35.8	10.8	-39.5	-18.3	18.1	-23.9	-24.0	6.3	-7.0	23.7	16.5	19.1	2.7	3.7				
-2.6	-36.4	12.9	-12.7	-6.6	0.1	12.6	4.6	-0.6	3.9	63.5	-17.4	20.1	0.1	2.4	-2.2	-0.1	132.7	-68.2	47.8	123.6	-62.0	-40.6	-15.2	
61.8	3.1	31.6	-1.7	-74.8	-8.4	95.6	-9.5	14.0	-2.3	-90.6	-45.7	72.6	-55.9	-29.6	14.9	6.0	44.7	38.4	0.1	3.5	6.9	2.5	3.0	
2.1	0.9	2.3	-0.5	1.4	2.7	2.1	-0.7	-0.7	4.2	-0.1	2.4	3.3	-1.0	0.7	7.2	0.5	-8.9	5.6	0.8	1.6	0.7	-2.0	0.1	
5.5	9.9	9.3	16.6	4.5	2.1	5.2	3.7	5.3	6.0	37.3	-3.3	-4.3	2.5	13.1	1.3									
tri-n-butylphosphine 2	-0.4	-17.6	1.9	-45.3	28.1	-8.5	-46.7	9.0	-43.1	-13.8	15.5	-24.9	-26.5	-1.1	-11.4	23.8	15.9	19.1	2.7	2.2				
-4.1	-42.9	8.5	-17.0	-11.7	-2.4	4.2	4.0	-8.1	4.7	62.9	-19.4	13.3	-5.2	-4.1	-4.7	0.3	127.2	-74.4	46.0	124.4	-66.0	-38.6	-16.4	
53.0	1.4	26.3	-8.0	-91.7	-19.5	98.5	-12.5	7.2	-10.2	-69.6	-30.1	78.1	-47.1	-18.8	6.3	9.2	54.8	46.1	-0.5	4.1	7.7	3.8	4.4	
3.1	2.9	4.5	5.0	7.2	8.3	7.7	7.0	4.9	8.0	7.6	7.8	9.4	1.8	2.3	9.2	7.6	-6.9	11.6	6.4	7.3	4.6	0.4	-1.7	
4.1	13.5	13.4	14.8	3.2	5.1	5.8	4.4	6.9	9.9	32.0	2.0	2.3	1.6	17.3	7.4									
tri-n-butylphosphine 3	-3.3	-19.2	-0.3	-40.9	26.5	-7.7	-34.9	16.4	-33.3	-9.0	24.3	-25.7	-28.1	-1.1	-11.9	24.0	14.7	17.7	0.0	-0.9				
-6.4	-45.3	3.6	-19.1	-15.9	-6.9	1.2	6.2	-6.6	5.6	57.9	-24.2	8.7	-6.0	-4.6	-6.2	-2.4	124.0	-71.6	41.9	125.5	-75.7	-45.9	-25.5	
55.9	-3.7	21.0	-8.1	-87.7	-21.9	91.4	-18.5	0.7	-14.7	-84.4	-43.0	76.4	-56.5	-28.9	5.6	-0.6	42.7	37.0	-5.2	-3.3	2.1	-1.5	-0.4	
-3.5	0.6	-0.1	-0.8	4.2	4.2	5.5	1.3	3.0	4.4	0.4	1.1	4.8	-2.0	-1.1	7.4	-0.4	-13.8	8.3	-0.9	4.8	2.6	4.2	5.2	
12.7	16.1	16.2	17.7	3.8	8.2	10.5	9.3	10.5	13.0	33.4	2.4	6.0	4.4	18.3	7.9									
tri-n-butylphosphine 4	1.2	-11.9	-0.6	-50.6	29.8	-15.1	-50.2	16.5	-45.9	-14.0	20.1	-33.6	-28.8	2.3	-8.7	25.0	16.6	22.1	4.7	4.4				
-4.1	-31.5	8.1	-8.0	-8.2	0.5	1.8	4.1	-9.5	6.1	59.5	-20.9	14.6	-2.3	0.2	-2.2	0.3	136.5	-55.7	51.8	133.5	-60.8	-44.2	-17.5	
65.7	0.1	27.2	-1.5	-75.7	-8.7	93.4	-19.9	9.4	-1.0	-85.5	-43.4	78.1	-51.3	-25.3	12.0	4.8	42.3	34.8	-1.1	1.4	5.1	0.4	2.5	
2.5	2.9	3.4	3.1	0.7	1.7	2.9	0.1	-0.5	4.2	1.5	2.4	7.0	-1.2	-1.3	7.6	0.0	-13.2	11.1	1.7	3.9	2.3	-1.8	-2.9	
4.6	12.8	12.3	11.9	3.6	5.0	7.4	6.3	8.2	11.2	35.6	2.3	4.3	4.2	18.6	7.7									
dimethylphenylphosphine AVG	4.4	-17.9	-3.3	-33.5	30.4	-27.1	-47.6	22.9	-41.8	-25.2	29.0	-64.2	-9.0	15.4	18.0	18.1	4.7	-5.5						
9.8	2.3	-9.6	-34.2	16.6	-7.0	-3.5	-0.6	-2.2	3.9	-5.3	1.4	55.1	-15.6	33.6	-3.0	-2.4	-16.2	0.8	146.0	3.3	36.2	105.7	-53.1	
0.4	0.3	36.4	0.7	22.2	-18.6	0.4	43.9	107.6	0.0	24.5	11.6	-18.0	-13.6	75.0	0.3	-3.8	28.4	3.3	102.0	110.3	0.0	20.6	20.0	
3.5	6.3	-6.6	1.4	4.4	-5.1	1.1	1.2	0.2	2.7	14.6	2.1	4.2	9.5	0.3	23.3	28.0	-7.9	-0.2	-9.2	3.8	-0.4	2.6	1.0	
-7.7	-7.0	-2.9	7.6	2.8	-0.7	-1.6	-6.3	-3.6	-4.2	-1.9	47.5	-4.6	-4.1	0.4	19.1	3.1								
dimethylphenylphosphine 1	0.1	-21.3	-7.6	-34.8	26.7	-30.0	-47.3	25.7	-40.6	-25.9	24.7	-66.3	-10.2	15.4	16.3	15.7	4.6	-5.1	8.3					
1.3	-9.5	-34.2	14.0	-6.7	-4.8	-2.9	-0.5	3.9	-7.1	1.5	55.2	-13.0	36.5	-1.6	-2.4	-15.5	1.1	147.4	9.2	36.5	106.3	-48.1	0.2	
0.4	35.5	0.2	22.8	-21.8	0.6	44.4	109.7	0.3	25.1	15.1	-15.4	-11.4	79.3	0.4	-0.8	31.3	5.2	105.0	114.6	0.2	22.2	20.9	3.7	
7.5	-5.7	2.7	4.2	-3.8	2.3	2.0	2.3	3.8	15.2	3.3	5.9	10.7	4.7	26.5	32.4	-7.4	0.0	-7.3	4.9	-0.4	3.7	0.2	-7.4	
-8.9	-2.9	3.9	1.3	-1																				

1-Myrtenal 1	-6.6	-1.5	-0.9	-17.2	2.9	2.6	-28.1	-8.7	-23.4	-26.5	-23.1	-10.3	-17.9	-12.9	-8.4	-0.6	2.7	7.4	3.2	3.4	4.0		
-5.0	51.8	75.1	-10.9	-13.3	-3.1	-5.8	-2.9	-4.4	-4.8	-4.5	-3.1	-10.4	14.3	11.4	-1.6	16.2	8.7	-1.8	9.5	5.2	-2.7	-0.3	13.1
-1.7	-3.7	13.8	-2.0	1.2	8.5	0.3	2.8	15.2	0.2	3.4	30.3	-0.7	19.7	21.9	-0.7	20.9	27.0	-0.2	-43.4	10.4	54.2	76.2	-28.9
10.5	26.9	-11.3	45.3	45.9	-13.1	1.0	69.3	24.4	13.5	57.6	12.4	43.7	67.6	2.7	0.6	9.2	121.0	0.5	9.6	7.3	18.6	25.6	1.0
113.5	98.2	41.1	2.8	26.5	32.6	42.6	45.7	31.6	0.5	25.1	0.5	1.2	0.6	-1.7									
1-Myrtenal AVG	-5.7	-3.1	-2.2	-11.4	5.2	2.7	-18.0	-1.6	-12.9	-14.2	-20.4	-0.6	-8.8	-8.3	-6.6	3.1	4.4	8.6	3.1	3.3	2.2		
-3.3	51.9	77.9	-9.7	-10.7	-3.0	-2.8	-4.3	-4.7	-3.1	-2.2	-2.6	-2.0	9.8	5.4	-0.5	16.2	11.5	-0.6	8.5	2.3	-4.9	-3.6	12.0
-7.1	-6.8	7.6	-3.8	-5.4	6.1	-2.4	-1.5	9.6	-0.1	1.8	22.3	0.4	15.9	17.7	-0.9	16.2	22.8	-0.2	-48.8	1.3	61.4	76.7	-36.4
13.1	26.7	-20.9	50.5	48.8	-11.7	1.0	70.2	17.0	15.3	64.8	11.5	47.8	73.4	1.2	0.6	10.3	122.7	0.3	4.2	5.2	19.7	27.2	2.9
114.6	96.4	40.2	3.0	16.7	20.4	32.9	27.0	18.4	3.2	21.3	0.1	1.7	2.6	-2.3									
(d,l)-2-PPA 3	-2.2	2.1	0.8	-6.2	3.7	-15.9	-3.5	-2.3	-5.7	-2.7	-5.2	7.1	-2.4	-0.8	7.4	0.7	-1.4	-4.6	0.0	0.7	0.7		
-16.3	17.1	20.9	1.6	-0.6	0.7	5.5	3.3	5.9	2.8	9.6	8.2	1.5	-1.5	5.2	0.2	28.7	33.3	-0.4	14.5	13.6	1.0	0.4	44.6
-0.3	14.6	47.5	-0.5	-1.9	24.8	-0.4	3.2	40.0	0.1	4.8	54.2	0.6	21.8	39.9	-3.8	-1.3	2.0	-1.2	-46.4	-0.1	72.2	85.0	-23.7
37.8	42.8	-13.3	53.3	54.2	-7.9	1.4	50.8	12.6	10.9	58.1	6.0	42.5	56.6	-2.3	0.0	2.3	113.7	0.8	-12.9	11.2	22.1	33.6	0.4
131.4	107.2	64.9	-1.0	9.2	29.8	9.9	13.7	3.4	4.8	10.5	1.6	0.7	-2.2	-16.0									
(d,l)-2-PPA 1	-8.1	-5.7	-6.4	-14.1	-1.2	-28.7	-13.7	-9.7	-14.7	-9.6	-15.0	-0.7	-9.3	-4.7	0.3	-2.3	-2.7	1.1	-4.5	-5.3	-0.1		
-27.5	6.0	14.4	-8.3	-11.7	-8.8	0.4	-2.3	2.0	-6.0	-1.9	2.3	3.1	3.4	6.1	-0.2	30.8	29.2	-5.4	23.5	10.6	-7.1	-1.0	50.8
-3.8	11.2	50.4	0.9	3.6	30.4	0.0	11.5	39.1	-2.5	3.8	69.5	1.2	25.7	73.5	-1.4	6.1	12.1	-0.5	-38.0	5.3	76.7	86.9	-18.5
34.0	40.2	-17.2	52.6	54.1	-9.5	1.3	61.9	21.2	13.5	59.7	12.5	43.8	63.9	-0.1	0.6	2.8	104.2	-0.1	-18.7	1.7	20.2	27.0	3.0
139.3	112.1	77.6	3.0	15.7	36.8	14.6	12.6	10.2	6.0	3.3	-1.1	-2.7	-14.3	-25.2									
(d,l)-2-PPA 2	0.1	0.2	-0.1	-2.2	3.3	-14.1	-3.5	-4.6	-6.9	-0.8	-12.0	3.5	-3.0	-1.1	1.4	-0.3	0.6	0.8	0.2	0.5	-1.9		
-14.8	12.8	16.7	-1.2	-2.5	-1.1	3.1	2.3	0.7	-3.7	-0.1	1.3	-2.2	-6.2	-1.8	0.0	25.7	32.5	-5.8	12.3	9.9	-0.3	0.6	52.4
0.9	17.6	49.0	0.1	-1.1	19.7	1.1	9.9	43.5	-2.1	2.0	57.9	-0.9	20.1	40.8	0.0	3.2	8.9	0.0	-46.1	0.2	82.7	94.0	-31.3
35.9	41.9	-18.0	60.0	59.5	-5.0	2.0	53.8	18.5	12.6	64.1	8.7	47.4	61.1	-6.2	1.1	7.7	112.0	-0.9	-10.9	2.2	29.5	42.4	16.1
134.5	111.9	63.7	-0.2	9.7	27.4	10.6	7.5	2.9	3.8	6.5	-1.5	-0.7	-9.4	-21.3									
(d,l)-2-PPA AVG	-3.4	-1.2	-1.9	-7.5	1.9	-19.5	-6.9	-5.5	-9.1	-4.3	-10.8	3.3	-4.9	-2.2	3.0	-0.6	-1.2	-0.9	-1.4	-1.4	-0.4		
-19.5	12.0	17.3	-2.6	-4.9	-3.0	3.0	1.1	2.9	-2.3	2.5	3.9	0.8	-1.4	3.2	0.0	28.4	31.7	-3.8	16.8	11.4	-2.1	0.0	49.3
-1.1	14.5	49.0	0.2	0.2	25.0	0.2	8.2	40.9	-1.5	3.5	60.6	0.3	22.5	51.4	-1.8	2.7	7.7	-0.6	-43.5	1.8	77.2	88.7	-24.5
35.9	41.6	-16.2	55.3	55.9	-7.5	1.5	55.5	17.4	12.4	60.6	9.1	44.6	60.5	-2.9	0.6	4.3	109.9	-0.1	-14.2	5.1	24.0	34.3	6.5
135.0	110.4	68.7	0.6	11.5	31.3	11.7	11.3	5.5	4.9	6.8	-0.3	-0.9	-8.6	-20.8									
Benzaldehyde 3	-7.8	2.5	-5.9	14.6	35.7	16.7	-6.5	0.5	-10.0	5.4	9.3	15.5	-10.1	-5.2	-2.5	24.1	25.1	15.3	8.7	11.8	8.6		
8.6	62.6	76.7	9.4	6.2	1.2	-0.9	-0.5	-0.7	7.6	11.2	3.1	6.8	19.4	15.0	0.4	9.5	13.2	-0.5	13.0	6.8	-1.6	-0.4	15.9
0.7	10.9	30.1	-0.1	2.0	10.9	1.0	6.3	16.8	-3.4	0.5	23.2	-0.9	9.8	16.1	-0.3	3.7	12.3	-0.3	-73.2	0.3	80.7	95.6	-44.3
31.2	43.5	-23.5	36.9	39.2	-8.4	3.2	57.4	22.2	11.4	56.5	2.7	46.3	67.3	5.3	-0.4	7.6	109.6	0.3	1.0	7.1	30.0	45.1	1.7
117.4	109.1	56.8	-2.8	9.5	24.9	8.5	3.2	3.9	0.0	8.8	1.0	2.7	-16.6	-36.4									
Benzaldehyde 1	-8.6	0.7	-2.5	13.0	34.4	12.9	-13.0	-1.2	-19.6	3.6	16.7	18.4	-10.3	-4.8	-1.5	15.3	17.4	14.0	10.5	14.3	6.2		
4.0	61.9	82.0	8.6	0.6	-3.7	-1.5	-1.5	-2.5	3.6	3.8	0.4	4.8	19.9	16.1	-0.6	8.6	13.0	-1.9	13.6	4.1	-2.0	-1.2	15.1
-1.1	5.6	29.5	-0.6	-0.8	3.4	-1.0	3.0	11.6	-0.2	1.2	29.1	1.4	11.2	23.1	-0.4	9.0	13.4	0.1	-75.9	7.2	90.1	103.3	-47.0
35.3	50.4	-24.1	56.0	58.6	-13.4	1.9	66.9	26.5	14.1	63.6	7.3	56.6	87.7	1.6	1.0	14.7	145.0	-0.1	0.9	9.1	34.0	46.4	10.4
129.3	114.3	68.0	1.9	18.7	34.2	21.2	50.9	29.7	0.8	22.7	0.1	2.4	-14.7	-44.3									
Benzaldehyde 2	-6.6	4.1	-16.0	16.6	32.4	15.9	-5.6	2.4	-6.9	9.8	15.5	23.8	-9.0	-4.9	6.0	14.3	15.7	11.8	8.8	11.4	6.0		
12.8	54.6	74.5	15.3	1.3	0.9	-0.2	-4.4	1.1	-0.2	3.0	0.8	6.3	25.5	18.1	-0.4	9.1	9.9	3.2	12.3	7.8	0.2	-0.1	14.8
-0.2	10.5	29.4	-0.2	0.8	7.2	-0.2	3.6	11.9	-4.4	-6.7	21.7	0.2	4.3	10.6	-0.6	4.6	10.3	-0.3	-75.3	-4.4	88.6	96.4	-53.6
34.5	53.6	-28.9	40.8	40.0	-27.4	2.3	56.7	5.6	15.3	62.1	-9.3	53.0	71.3	-0.5	-0.6	18.5	132.0	0.4	3.1	10.1	28.0	43.6	13.6
126.1	114.7	63.0	-7.7	3.9	15.0	12.0	20.1	13.5	2.0	10.0	-7.7	1.0	-8.6	-36.9									
Benzaldehyde AVG	-7.6	2.5	-8.1	14.7	34.2	15.2	-8.4	0.5	-12.2	6.3	13.8	19.2	-9.8	-5.0	0.6	17.9	19.4	13.7	9.3	12.5			
7.0	8.5	59.7	77.7	11.1	2.7	-0.6	0.9	-2.1	0.7	3.6	6.0	1.4	6.0	21.6	16.4	-0.2	9.1	12.0	0.3	13.0	6.2	-1.2	-0.6
15.3	-0.2	9.0	29.7	-0.3	0.6	7.2	-0.1	4.3	13.4	-2.7	-1.7	24.7	0.2	8.4	16.6	-0.4	5.8	12.0	-0.2	-74.8	1.0	86.5	98.4
-48.3	33.7	49.2	-25.5	44.6	45.9	-16.4	2.4	60.3	18.1	13.6	60.8	0.2	52.0	75.4	2.1	0.0	13.6	128.9	0.2	1.7	8.8	30.7	45.0
8.5	124.3	112.7	62.6	-2.9	10.7	24.7	13.9	24.7	15.7	0.9	13.8	-2.2	2.1	-13.3	-39.2								
o-Tolualdehyde 2	-0.2	-1.5	3.2	-1.2	9.2	6.3	-14.3	-1.3	-21.4	-2.0	5.9	9.1	14.1	16.6	19.5	11.8	11.5	13.2	6.8	9.5	9.1		
5.2	56.5	64.8	4.5	-0.9	-3.9	0.0	-0.6	-1.3	6.3	12.5	7.9	11.6	13.4	16.8	-0.1	17.3	18.2	-1.9	14.0	1.6	-0.5	-0.2	15.4
0.1	4.2	16.8	0.4	1.1	2.8	0.7	2.0	16.3	-0.6	3.2	24.8	-0.1	12.6	19.2	0.2	12.9	19.0	-1.5	-46.4	-5.8	49.6	51.1	-38.1
15.7	22.7	-17.2	32.2	32.3	-1.2	2.3	61.1	15.5	18.7	62.5	-2.3	47.8	62.8	-6.0	-0.2	5.8	70.3	-0.2	1.2	3.7	26.9	30.6	2.7
92.2	85.7	53.2	2.1	9.8	20.4	30.2	22.5	20.1	6.0	19.9	-0.2	1.6	-8.5	-20.0									
o-Tolualdehyde 1	0.0	-1.																					

65.4	0.8	22.5	55.5	0.0	12.6	0.5	-0.5	16.2	49.0	-0.5	3.9	45.3	1.0	35.4	48.8	-0.5	9.8	8.0	-0.4	-45.9	-9.3	54.2	54.3	
-48.8	19.1	25.1	-30.9	18.8	16.9	-7.0	3.5	66.9	4.8	28.7	86.3	-17.0	60.3	79.8	-15.0	1.3	20.9	70.5	0.2	2.7	-2.8	19.5	24.2	
4.9	104.1	76.7	40.9	1.1	6.8	10.6	29.0	21.4	3.2	0.1	5.2	-0.4	0.0	1.3	-4.1									
Hexanal 1	-3.5	1.3	-0.2	-0.1	10.4	-14.2	-18.6	12.4	-32.1	0.0	2.6	9.8	0.6	4.1	1.8	-0.4	-0.7	1.4	5.7	4.0	8.3	18.0		
70.7	92.5	6.9	4.7	9.1	3.9	-1.0	9.8	1.9	1.4	0.0	-1.7	1.7	8.6	0.4	31.3	32.9	7.0	15.2	13.9	-0.5	0.4	58.5	-0.1	
13.9	40.6	-0.1	4.7	-2.2	-3.1	7.4	33.6	1.0	3.7	23.5	0.5	27.0	24.4	0.7	8.3	5.4	0.0	-61.4	-17.8	65.4	67.1	-64.8	22.1	
30.6	-42.6	32.6	30.1	-14.7	1.5	65.2	5.5	26.3	82.4	-18.1	54.5	66.2	-14.8	-1.5	19.6	95.0	1.0	1.6	3.0	17.9	20.9	2.7	100.9	
80.9	38.7	0.7	13.6	8.9	23.1	20.4	4.6	0.8	10.0	0.4	0.5	20.7	23.1											
Hexanal 3	2.3	4.1	3.3	-0.8	7.4	-5.1	-12.3	11.6	-21.1	-5.5	4.3	6.5	1.4	5.5	2.7	1.0	1.9	2.3	1.9	4.1	2.8	17.2		
75.0	86.4	2.6	1.7	4.4	1.2	0.6	6.4	3.3	1.8	3.1	4.2	3.7	7.2	0.3	27.9	21.5	2.6	12.0	5.8	1.1	0.4	46.9	0.8	
14.6	35.2	0.0	10.7	1.8	0.7	10.7	37.1	-0.9	2.2	38.7	-0.2	24.6	28.6	-0.3	6.5	7.0	0.9	-58.2	-15.0	72.1	75.7	-57.0	28.7	
34.9	-43.1	25.0	26.8	-12.4	1.9	69.4	10.4	26.9	87.4	-12.1	54.1	78.5	-14.9	0.0	12.1	105.2	-0.4	2.1	-0.1	24.4	25.2	3.5	105.4	
83.2	36.2	1.6	20.5	17.5	30.0	22.9	5.9	0.4	9.6	-1.1	0.6	9.9	10.9											
Hexanal 4	6.2	7.3	9.5	-1.2	10.7	-6.0	-13.0	12.9	-16.7	0.6	4.2	8.1	1.5	6.8	6.9	1.8	3.2	4.7	4.7	4.8	4.0	21.0		
82.1	101.5	1.3	-0.3	8.9	1.0	-4.2	5.4	1.7	3.2	3.3	2.9	3.5	10.2	-1.0	29.9	28.9	5.8	13.5	13.4	0.8	1.5	54.7	0.3	
11.1	33.7	0.0	7.7	1.0	0.8	10.7	37.3	-0.8	7.6	38.2	-0.2	26.2	28.2	0.1	8.5	9.4	-1.1	-53.2	-8.9	72.4	73.2	-54.1	23.4	
33.2	-38.8	28.3	26.6	-14.3	5.3	65.4	4.4	30.4	87.4	-12.8	60.5	83.4	-11.7	0.8	25.3	109.2	0.9	3.6	0.0	23.1	30.8	9.0	110.8	
87.7	44.0	5.1	13.8	14.5	34.5	26.3	-2.3	1.4	10.3	1.0	-1.0	13.5	14.1											
Hexanal AVG	1.7	4.2	4.2	-0.7	9.5	-8.4	-14.6	12.3	-23.3	-1.6	3.7	8.1	1.2	5.5	3.8	0.8	1.5	2.8	4.1	4.3	5.0			
18.8	76.0	93.5	3.6	2.0	7.5	-2.1	-1.5	7.2	2.3	2.1	2.1	2.9	8.7	-0.1	29.7	27.8	5.1	13.6	11.0	0.5	0.7	53.3		
0.3	13.2	36.5	0.0	7.7	0.2	-0.5	9.6	36.0	-0.2	4.5	33.5	0.0	26.0	27.1	0.2	7.7	7.2	-0.1	-57.6	-13.9	70.0	72.0	-58.6	
24.7	32.9	-41.5	28.6	27.8	-13.8	2.9	66.7	6.8	27.9	85.7	-14.4	56.4	76.0	-13.8	-0.2	19.0	103.2	0.5	2.4	1.0	21.8	25.6	5.1	
105.7	83.9	39.7	2.5	16.0	13.6	29.2	23.2	2.8	0.9	10.0	0.1	0.0	14.7	16.1										
Octylaldehyde 3	-6.2	-1.1	-2.4	-14.6	1.3	-6.2	-18.2	3.5	-29.6	-10.6	-2.0	0.8	-0.5	-0.7	2.1	-6.7	-2.7	1.1	-1.0	-0.2	3.2			
9.3	63.3	82.5	-2.8	-4.6	-1.3	-1.7	-4.0	1.8	-4.2	1.4	-2.6	-2.3	-1.7	1.2	-0.9	19.8	18.1	-0.1	13.7	7.4	1.4	0.6	38.2	
0.7	13.0	41.8	0.2	9.1	3.5	1.2	2.3	29.7	-3.2	3.6	17.4	-0.1	20.3	19.9	-0.2	9.8	15.2	0.0	-61.7	-9.0	89.0	90.0	-49.2	
35.2	46.0	-45.4	37.6	35.6	-12.0	4.2	75.9	12.5	29.3	89.7	-8.3	58.4	84.7	-7.0	1.6	13.6	110.9	0.9	7.4	1.7	21.1	22.1	1.4	
99.5	66.5	33.2	3.1	26.9	20.8	36.1	46.5	3.0	0.0	16.5	0.4	0.2	17.0	20.1										
Octylaldehyde 2	0.2	4.5	-5.9	8.9	1.5	-11.6	-19.4	7.9	-38.1	-6.7	1.4	2.1	0.7	1.8	0.7	-0.1	-0.4	5.9	0.8	0.7	1.3			
15.1	67.4	91.7	1.8	-1.6	6.0	1.1	-0.7	0.5	1.1	2.4	-1.5	0.7	1.6	4.3	-0.5	13.5	10.6	1.6	5.9	3.4	0.7	0.0	25.2	
1.8	9.9	36.2	0.5	9.1	-0.1	0.7	7.1	17.2	-1.6	2.3	13.7	0.3	13.5	11.9	-0.8	2.2	4.6	-1.0	-65.7	-22.1	81.4	82.0	-57.5	
29.9	38.3	-44.9	49.1	43.0	-25.8	7.5	64.1	6.9	29.8	82.0	-19.1	55.9	70.5	-17.0	0.3	19.2	102.1	1.2	-1.7	-2.7	20.6	23.0	7.7	
93.8	63.8	43.0	3.8	20.9	16.3	34.1	45.6	-4.5	0.4	2.8	0.1	0.2	3.5	5.7										
Octylaldehyde 4	-3.7	-2.8	-3.3	-9.0	4.1	-9.9	-15.1	5.1	-27.1	-2.4	0.5	2.5	-0.4	3.3	1.6	-0.4	-1.0	5.4	0.6	2.1	5.4			
17.6	76.3	100.2	1.4	-1.1	9.2	1.9	-1.3	4.4	-4.2	4.3	3.0	2.8	2.9	7.0	-0.6	18.3	20.9	-0.1	10.7	12.8	0.5	0.5	42.2	
0.6	13.2	34.3	-0.7	9.4	0.7	-0.8	11.2	28.4	0.6	6.4	22.4	-0.2	16.5	17.0	0.4	3.4	7.8	-1.0	-63.6	-14.9	82.5	82.0	-58.3	
28.1	39.6	-45.9	38.9	33.5	-19.5	5.3	68.3	7.3	30.3	90.2	-15.8	61.3	76.0	-14.9	-0.2	23.5	102.0	1.1	2.1	1.1	18.5	24.7	6.8	
107.7	77.0	48.5	4.0	18.7	13.6	39.3	31.1	-5.8	0.0	4.5	0.4	1.1	7.3	15.6										
Octylaldehyde AVG	-3.2	0.2	-3.9	-4.9	2.3	-9.2	-17.6	5.5	-31.6	-6.6	0.0	1.8	-0.1	1.5	1.5	-2.4	-1.4	4.1	0.2	0.9				
3.3	14.0	69.0	91.5	0.1	-2.4	4.7	0.4	-2.0	2.2	-2.4	2.7	-0.3	0.4	0.9	4.2	-0.7	17.2	16.5	0.5	10.1	7.9	0.8	0.4	
35.2	1.0	12.0	37.5	0.0	9.2	1.4	0.4	6.9	25.1	-1.4	4.1	17.8	0.0	16.8	16.2	-0.2	5.1	9.2	-0.7	-63.7	-15.3	84.3	84.7	
-55.0	31.1	41.3	-45.4	41.9	37.3	-19.1	5.7	69.5	8.9	29.8	87.3	-14.4	58.6	77.1	-13.0	0.6	18.8	105.0	1.1	2.6	0.1	20.1	23.3	
5.3	100.3	69.1	41.6	3.6	22.2	16.9	36.5	41.1	-2.4	0.1	8.0	0.3	0.5	9.3	13.8									
Decylaldehyde 4	-0.7	0.0	0.5	-6.9	4.1	8.0	-3.6	-1.2	-1.0	-11.0	8.8	5.5	-1.2	-0.4	2.8	0.4	0.8	1.7	-1.4	-1.2	-1.0			
-6.0	57.0	79.0	-6.6	-5.9	-5.7	0.1	0.6	0.9	-6.4	-1.1	-0.3	-7.1	-4.9	-3.1	-0.9	12.2	2.6	-1.6	11.4	0.8	-8.3	-4.0	6.6	
-6.2	2.1	24.9	-1.1	1.6	8.7	-3.4	-2.5	7.6	0.4	1.0	24.9	0.6	3.1	15.0	-0.4	3.6	7.3	-1.1	-54.7	4.7	78.1	89.8	-42.0	
32.9	44.0	-23.5	35.0	31.9	-10.0	1.4	68.0	19.9	15.3	62.2	0.9	52.0	77.8	1.5	1.1	4.4	132.3	-1.2	9.4	13.1	28.6	39.6	2.7	
118.7	108.4	52.3	2.6	14.7	20.6	18.9	9.2	4.6	0.3	12.0	-0.7	0.0	0.4	-0.9	-0.9									
Decylaldehyde 1	-1.3	1.3	-1.8	-6.8	3.0	9.4	-7.2	-6.0	-9.1	-8.7	0.7	2.8	-5.3	-1.8	-1.2	3.5	6.2	5.4	-0.6	0.7	-0.2			
0.1	59.3	81.8	-2.2	-1.5	0.9	1.8	2.2	2.2	-3.8	2.8	-0.4	-1.9	-4.2	-1.2	-0.2	12.4	1.0	2.4	7.7	1.2	-3.8	-1.6	7.6	
-4.1	2.9	18.5	-0.2	4.8	5.9	-1.2	0.7	12.8	0.0	-0.4	16.0	-1.0	5.5	7.8	0.3	4.9	2.8	-1.0	-56.7	0.4	74.4	83.1	-47.2	
24.7	35.4	-30.7	29.9	27.6	-16.0	-0.7	56.2	11.9	14.9	63.0	-7.4	49.9	71.0	2.0	0.5	15.1	106.9	0.2	-2.0	6.6	23.8	35.5	3.5	
120.2	108.1	44.5	0.9	8.2	8.1	18.2	6.8	-1.7	-2.4	2.5	-4.3	-7.0	-7.3	-7.8										
Decylaldehyde 2	0.2	-1.4	-4.0	-5.5	3.3	7.7	-0.3	-5.6	-5.7	-9.2	1.8	-0.1	-2.0	-0.9	0.0	-8.4	-9.2	-11.9	1.5	2.3	-1.9			
2.0	59.0	80.2	0.6	-0.3	-5.7	-5.5	-4.6	-4.4	1.0	-1.4	-3.9	-6.4	-0.6	0.7	14.5	5.7	4.1	11.6	-0.2	-2.6	0.7	7.1		
-1.0	3.9	18.8	0.7	6.0	9.4	-3.0	1.7	12.5	-1.8	-3.6	13.0	0.4	1.7	10.4	-0.9	2.9	8.7	0.1</						

19.0	23.1	-19.1	21.2	23.3	-10.8	1.7	47.2	2.2	10.4	53.0	-6.1	45.1	60.3	-1.4	1.2	15.0	84.8	0.9	3.0	-0.2	19.5	29.6	5.5	
123.7	101.5	56.1	-2.0	-0.1	2.9	32.5	12.8	5.3	1.2	7.8	0.8	2.7	-4.0	-23.8										
Nonylaldehyde 3	-4.1	-0.3	-0.8	-6.1	11.0	13.6	-28.3	2.4	-33.5	-14.3	-12.4	2.1	16.7	31.3	37.6	12.3	15.3	17.9	8.1	7.9	11.9			
0.4	48.2	60.6	3.4	2.0	12.8	1.7	-0.4	9.3	5.5	11.2	9.9	1.1	10.1	20.5	2.1	48.2	41.5	13.7	35.2	16.0	-2.6	0.9	60.5	
-0.6	21.1	69.4	0.5	7.0	5.9	0.8	8.2	67.1	-0.5	8.3	59.2	2.5	31.2	69.8	-0.1	10.2	15.4	-0.1	-40.8	2.2	57.7	64.1	-30.3	
19.1	24.3	-16.4	27.4	26.6	-7.3	2.1	57.2	10.4	17.5	57.7	-1.4	50.0	67.7	1.7	-1.1	11.2	103.4	0.4	5.4	-1.9	24.8	24.1	1.0	
125.5	104.2	55.0	3.3	8.2	17.1	33.0	17.2	9.5	1.9	11.5	-0.1	3.6	-3.4	-14.0										
Nonylaldehyde AVG	-1.8	-0.8	-1.2	-5.2	10.8	11.8	-20.6	1.6	-27.9	-9.2	-10.6	5.8	18.6	33.1	37.8	10.6	13.4	14.8	9.5	8.0				
8.8	1.1	47.0	65.2	1.6	-0.4	9.5	0.4	-1.9	5.1	4.0	9.3	7.2	1.9	9.4	18.3	1.0	48.7	38.7	13.9	35.2	18.6	-0.6	0.6	
62.4	0.2	20.8	73.0	0.1	8.0	3.1	0.7	10.2	65.2	-2.6	5.6	58.1	1.5	28.4	71.6	0.5	6.3	11.9	0.0	-43.0	-0.6	54.3	59.7	
-33.5	17.7	21.7	-18.4	25.0	25.7	-11.5	2.2	50.9	7.9	14.8	54.3	-3.9	47.5	62.6	-0.6	0.3	14.3	85.8	0.4	2.9	-2.0	22.0	26.2	
3.3	126.3	102.8	58.2	0.1	4.3	11.2	30.7	14.1	7.2	1.1	8.1	0.2	3.0	-5.8	-21.0									
Ethyl benzoate 2	4.1	0.7	0.7	-0.7	5.0	10.9	-2.3	-2.6	-4.9	-3.5	-4.9	1.5	8.7	15.2	19.6	10.9	11.6	12.3	7.1	7.1	8.5			
-0.1	-1.7	1.2	-4.5	-3.3	2.7	2.7	-5.3	10.1	6.3	6.5	4.5	4.7	11.1	17.8	-0.3	17.7	14.1	3.6	9.0	2.5	-0.1	-0.1	14.4	
0.3	-0.6	10.3	-0.6	-0.1	4.7	0.3	5.0	17.1	-0.8	1.4	9.0	0.2	10.1	12.4	-0.4	11.1	16.6	-0.2	-12.9	7.0	14.1	15.5	-15.0	
8.3	7.6	-8.9	7.5	5.4	2.5	1.7	34.2	8.6	13.3	43.0	2.5	36.7	45.5	0.3	-0.6	9.7	10.6	-0.5	-0.7	4.6	13.5	21.4	6.8	
101.1	19.3	60.8	-0.6	2.0	10.4	21.8	15.1	21.0	1.6	13.1	0.6	0.5	-2.7	-9.9										
Ethyl benzoate 1	-3.3	-4.2	-5.0	-1.7	10.3	12.2	-8.9	-2.0	-9.0	-10.5	-9.4	-8.4	3.7	11.8	16.7	5.7	5.9	12.3	12.3	10.8	13.7			
-7.0	-4.0	0.5	-6.6	-7.4	-0.9	2.8	-6.9	11.0	4.4	4.4	5.5	-1.8	4.7	13.4	0.3	17.1	13.2	2.7	9.0	6.8	-2.9	-2.5	17.0	
-3.2	0.7	11.0	0.0	-2.1	6.8	-1.3	1.2	19.3	0.9	4.2	16.5	0.5	10.3	15.9	0.7	11.7	20.4	0.3	-11.6	10.2	15.2	18.7	-8.4	
8.1	10.6	-3.5	10.6	10.9	7.7	2.4	42.0	12.2	18.3	45.6	6.4	33.9	45.0	5.6	1.3	12.2	15.8	0.1	2.6	5.2	17.1	23.3	4.0	
89.5	90.4	55.1	2.1	6.6	18.5	13.9	0.1	18.2	-0.1	14.3	0.5	1.5	3.3	2.1										
Ethyl benzoate 3	-1.0	0.6	0.3	-6.3	7.1	9.4	-11.3	-2.2	-9.3	-11.0	-2.0	-1.7	6.5	14.6	18.7	11.9	14.1	14.8	8.9	11.6	8.2			
-3.1	4.2	7.8	-1.6	-1.1	4.8	0.0	-6.5	7.9	6.5	5.2	3.6	-0.5	6.2	12.1	-0.8	22.6	21.2	7.5	14.4	6.9	-0.8	1.2	24.3	
-0.2	3.9	13.7	-0.1	-3.2	0.0	-0.8	-2.5	6.2	0.4	2.2	15.4	0.9	17.6	15.2	0.5	17.6	22.7	0.2	-5.7	9.3	16.1	22.4	-6.7	
9.3	15.4	-3.7	4.2	4.3	0.3	0.9	28.5	7.6	15.3	40.3	6.7	34.0	44.6	4.7	0.9	3.3	23.9	-0.4	7.4	-0.1	11.0	16.4	0.4	
80.7	78.0	47.7	0.6	3.3	10.2	21.0	18.2	25.3	-0.5	22.3	0.3	-0.2	5.6	-0.1										
Ethyl benzoate AVG	-0.1	-1.0	-1.3	-2.9	7.5	10.8	-7.5	-2.3	-7.7	-8.3	-5.4	-2.9	6.3	13.9	18.3	9.5	10.6	13.2	9.4	9.8				
10.1	-3.4	-0.5	3.1	-4.2	-3.9	2.2	1.8	-6.2	9.7	5.7	5.4	4.5	0.8	7.3	14.4	-0.3	19.1	16.2	4.6	10.8	5.4	-1.3	-0.5	
18.6	-1.0	1.3	11.7	-0.2	-1.8	3.9	-0.6	1.2	14.2	0.2	2.6	13.7	0.5	12.7	14.5	0.3	13.4	19.9	0.1	-10.1	8.8	15.1	18.9	
-10.0	8.6	11.2	-5.4	7.4	6.9	3.5	1.7	34.9	9.5	15.6	43.0	5.2	34.9	45.0	3.5	0.5	8.4	16.8	-0.3	3.1	3.3	13.9	20.4	
3.7	90.4	86.6	54.5	0.7	4.0	13.0	18.9	11.1	21.5	0.3	16.6	0.5	0.6	2.1	-2.6									
Methyl benzoate 3	-3.1	-2.1	-0.7	0.2	9.3	13.3	-10.2	-6.3	-5.1	-8.0	-14.6	4.4	20.0	37.1	44.0	14.8	19.0	16.7	7.6	9.8				
10.6	-5.8	1.2	5.7	-1.2	-0.8	9.1	-0.9	-3.3	1.9	11.8	12.7	11.7	2.1	8.5	15.4	-0.3	11.5	15.8	-0.4	8.4	7.1	-1.9	0.5	
18.4	1.0	3.4	12.1	0.3	-0.4	3.4	-0.4	0.7	7.6	-3.3	2.6	15.9	0.3	10.4	10.6	-0.9	9.4	22.7	-0.3	-1.4	11.2	6.2	10.2	
-0.9	2.5	4.2	-1.4	6.6	5.4	10.3	2.1	19.2	12.0	9.0	23.8	7.9	20.0	28.0	8.1	-0.4	6.2	10.9	-0.9	7.1	3.4	3.4	10.5	
-0.4	36.7	49.8	38.3	0.7	2.5	16.4	20.3	13.3	20.4	0.4	16.5	0.5	0.8	1.2	-5.4									
Methyl benzoate 4	0.9	1.7	5.5	10.0	17.4	19.1	-1.2	7.4	3.8	1.8	-12.8	9.2	26.2	40.5	42.1	20.4	20.8	16.1	13.5	14.1				
13.0	1.0	5.8	11.8	6.6	7.2	14.1	0.1	-2.5	0.3	15.4	13.7	12.9	5.5	10.4	17.8	0.7	12.4	15.3	4.8	6.2	7.0	0.0	0.4	
16.5	1.0	7.2	9.9	-0.5	1.2	2.6	-1.3	2.8	12.0	-1.7	1.6	11.4	-0.5	7.6	7.4	0.3	7.4	16.8	-1.2	-3.3	5.0	5.0	5.9	
-6.5	4.3	3.0	-2.6	2.7	2.0	1.2	1.9	17.1	6.4	5.3	18.3	-0.6	15.5	21.5	0.0	-1.0	6.9	4.6	0.8	7.2	1.7	2.2	5.7	
1.7	43.1	51.6	36.8	-0.1	-8.5	5.4	17.9	7.2	11.0	2.0	7.2	-0.3	0.1	-5.6	-15.3									
Methyl benzoate AVG	-1.1	-0.2	2.4	5.1	13.3	16.2	-5.7	0.6	-0.7	-3.1	-13.7	6.8	23.1	38.8	43.0	17.6	19.9	16.4	10.5	11.9				
11.8	-2.4	3.5	8.8	2.7	3.2	11.6	-0.4	-2.9	1.1	13.6	13.2	12.3	3.8	9.4	16.6	0.2	12.0	15.5	2.2	7.3	7.0	-1.0	0.4	
17.4	1.0	5.3	11.0	-0.1	0.4	3.0	-0.8	1.8	9.8	-2.5	2.1	13.6	-0.1	9.0	9.0	-0.3	8.4	19.8	-0.8	-2.3	8.1	5.6	8.1	
-3.7	3.4	3.6	-2.0	4.6	3.7	5.8	2.0	18.1	9.2	7.2	21.0	3.6	17.8	24.7	4.0	-0.7	6.6	7.7	-0.1	7.1	2.5	2.8	8.1	
0.7	39.9	50.7	37.5	0.3	-3.0	10.9	19.1	10.3	15.7	1.2	11.8	0.1	0.4	-2.2	-10.4									
Ethyl nonanoate 1	-1.6	-1.2	3.0	3.0	6.5	12.9	-3.3	3.0	1.8	-0.1	-12.5	14.9	2.6	8.4	10.4	3.4	6.4	10.8	7.1	8.2	7.2			
3.2	9.7	10.6	6.3	4.6	12.4	3.0	-1.3	9.7	3.5	7.3	7.0	0.6	5.6	13.5	0.6	4.0	-0.4	4.3	3.8	1.7	0.6	0.2	2.7	
-0.3	6.6	1.9	0.9	2.3	0.9	0.9	1.7	-4.0	1.9	2.4	0.9	-0.7	4.1	2.8	-1.1	8.9	4.0	-0.1	7.7	2.4	0.4	-1.2	11.8	
-1.5	2.0	0.0	0.1	2.5	5.3	1.8	-9.6	0.6	-4.2	-6.1	2.6	-14.6	-13.6	6.3	-0.6	3.5	1.3	-0.1	1.9	4.0	-3.5	-1.3	1.9	
Ethyl nonanoate AVG	-2.2	-1.0	1.1	-1.0	4.2	11.2	-5.2	0.7	2.3	-2.2	-17.5	9.9	3.4	9.1	11.2	4.6	8.4	11.5	5.9	7.9				
6.8	-0.6	5.0	10.0	1.1	0.2	8.4	1.1	-2.8	12.0	4.6	6.8	7.0	2.2	7.1	14.1	0.1	5.1	1.3	3.1	3.2	1.1	-1.8	-1.2	
-1.3	-1.9	0.7	2.1	0.4	-0.7	1.6	-0.3	1.1	-5.9	3.5	4.0	1.7	-0.5	3.1	2.8	-1.3	8.1	4.8	-0.9	2.0	1.7	-2.3	-0.7	
6.2	0.1	1.8	0.2	0.6	2.8	5.0	1.2	-6.6	3.5	-1.0	-3.3	8.1	-12.1	-11.4	8.7	-1.1	1.9	2.6	-0.8	1.3	4.1	-1.9	0.0	
3.8	0.9	2.0	2.7	3.3	6.9	6.8	2.2	6.7	8.3	5.														

Methyl octanoate 3		0.4	2.9	3.3	3.8	13.1	21.5	-12.5	-0.8	0.1	-7.3	-3.7	16.6	11.8	24.4	27.6	11.3	15.0	21.4	13.5	14.1		
12.2	3.8	13.8	13.5	8.1	11.9	17.7	-2.2	-3.5	0.3	4.1	8.0	3.5	-1.5	9.7	16.8	0.1	7.2	4.8	9.9	2.4	4.9	-0.2	10.4
12.4	-1.5	20.9	74.9	-0.4	-3.5	0.2	0.3	5.2	4.3	2.3	4.2	1.4	0.6	4.6	-0.6	-0.6	12.0	5.8	6.1	8.3	12.1	-0.2	3.8
9.9	-4.7	-1.0	-2.9	-1.3	-0.7	-0.3	-0.7	-2.9	-0.6	0.5	1.8	4.0	3.4	3.7	13.6	-0.5	11.8	11.1	-0.7	0.3	1.0	4.8	6.3
1.9	5.3	1.9	8.9	2.0	2.1	0.3	10.9	10.3	2.9	15.6	24.7	-1.7	0.4	22.5	31.5								
Methyl octanoate AVG		-1.9	-0.7	-0.4	2.2	11.5	18.4	-8.9	0.2	1.6	-2.1	-1.2	19.7	12.9	23.1	24.3	10.6	14.2	18.0	11.5	12.7		
10.2	0.3	8.9	12.0	7.0	8.6	15.2	1.9	-1.6	4.5	7.4	9.3	8.0	2.1	8.7	15.7	0.4	6.8	3.2	8.4	2.5	2.7	-0.3	5.6
9.1	-0.1	19.5	71.8	0.7	-1.0	2.3	-1.4	5.8	5.2	1.9	4.7	3.6	0.4	7.0	2.5	-0.6	9.3	6.5	2.6	4.7	4.9	-0.2	2.7
6.3	-1.0	0.8	0.9	2.0	2.3	5.7	1.0	-2.2	3.0	0.4	0.8	3.7	-1.9	-2.0	9.0	-1.2	5.1	6.1	-1.1	1.2	1.5	8.0	7.1
6.9	8.8	4.4	10.4	1.9	3.8	2.6	7.6	6.1	0.7	5.0	12.8	-0.2	0.7	16.2	21.7								
1-octanethiol 2		0.6	-0.4	-0.6	6.7	12.6	33.2	-7.2	-4.1	-6.8	-26.9	14.0	2.2	5.9	13.5	17.3	-10.4	-4.9	10.7	18.5	18.7	15.5	
-1.0	17.8	19.6	5.0	12.0	2.7	-0.8	-3.6	4.1	8.4	13.9	5.4	0.7	9.6	15.1	0.2	3.0	9.9	0.7	1.8	2.0	-0.2	1.2	4.9
-0.9	5.3	12.4	-0.5	-0.1	3.3	0.2	3.8	7.4	0.5	1.3	5.1	-0.5	2.7	0.7	-1.4	2.8	4.4	0.0	-3.9	1.4	0.9	2.4	-5.9
1.4	2.5	-0.6	2.2	2.9	3.4	5.0	7.9	2.0	5.5	7.2	1.0	8.8	8.4	0.7	0.5	-0.7	2.4	1.8	-1.3	-4.6	3.7	5.3	3.0
10.6	8.6	11.1	1.7	5.0	4.2	1.6	0.9	0.7	0.0	5.4	1.1	0.3	6.5	13.5									
1-octanethiol 1		-5.5	-5.2	-5.3	6.8	11.0	29.9	-10.4	-1.8	-9.1	-25.2	2.2	-1.1	12.3	21.8	31.3	-4.9	12.1	22.7	19.0	17.5	14.7	
-1.5	15.2	19.6	2.8	8.9	2.1	1.2	-3.0	6.0	9.5	12.4	4.8	-0.1	7.4	10.7	-1.8	1.9	10.8	-0.3	0.1	3.7	-0.5	-4.3	6.8
-0.6	1.4	3.3	-0.2	-0.6	3.7	0.3	4.9	7.6	1.1	6.1	4.0	0.6	4.8	5.7	1.0	4.9	7.0	0.1	-2.7	4.5	3.8	4.6	0.2
4.7	3.9	3.3	5.2	4.6	5.6	5.8	11.8	4.1	9.0	11.6	-0.3	9.1	11.5	-0.6	0.2	1.8	3.8	3.2	0.2	-2.8	8.2	8.6	9.4
8.3	8.5	10.7	4.5	5.0	5.8	2.4	3.7	1.9	0.0	5.9	4.5	-0.4	9.0	13.8									
1-octanethiol 3		-0.1	-1.7	0.1	4.7	11.8	30.7	-10.3	-2.7	-10.3	-26.0	6.5	-1.6	14.2	24.5	32.1	-7.9	8.3	18.9	12.8	15.1	10.8	
-0.8	14.1	17.0	4.1	6.8	4.7	-1.1	-4.8	1.7	7.7	10.5	4.6	-2.8	8.3	10.0	-0.7	3.1	10.8	1.7	0.6	2.3	-0.5	0.3	9.6
0.4	4.4	11.1	-0.4	-1.4	2.5	0.1	3.5	5.8	2.4	0.8	5.6	0.7	3.6	3.7	3.6	3.0	3.9	1.6	0.2	0.8	1.0	2.0	2.7
3.0	3.0	2.0	0.5	0.8	1.8	6.9	8.4	1.6	7.3	6.7	-0.5	8.4	9.5	-2.9	0.0	1.8	0.8	3.8	-0.2	-7.5	5.0	4.6	4.8
Avg 1-octanethiol		-1.7	-2.4	-1.9	6.1	11.8	31.3	-9.3	-2.9	-8.7	-26.0	7.6	-0.1	10.8	19.9	26.9	-7.8	5.2	17.5	16.8	17.1		
13.7	-1.1	15.7	18.8	4.0	9.3	3.2	-0.2	-3.8	3.9	8.5	12.3	4.9	-0.8	8.4	11.9	-0.8	2.6	10.5	0.7	0.8	2.7	-0.4	-0.9
7.1	-0.3	3.7	8.9	-0.4	-0.7	3.2	0.2	4.0	6.9	1.3	2.7	4.9	0.3	3.7	3.4	1.1	3.6	5.1	0.6	-2.1	2.3	1.9	3.0
5.7	8.4	8.2	9.7	2.4	4.2	4.7	1.4	1.3	-0.3	-0.1	5.3	3.1	0.0	7.7	13.8								
dodecane 1		-1.1	1.2	-0.5	2.0	6.6	3.5	-0.4	2.6	2.4	-2.4	-0.8	1.7	10.0	11.8	11.9	3.0	9.1	7.0	8.4	10.1	3.5	1.5
9.5	11.0	5.9	6.5	2.8	0.4	1.5	1.6	3.0	8.4	3.8	-1.4	-1.5	5.9	1.7	4.6	-1.8	-0.7	3.3	1.5	0.1	1.4	4.6	1.4
4.0	8.4	1.0	1.8	1.0	0.0	0.9	7.6	0.0	1.0	4.6	1.0	0.2	9.7	-1.6	7.8	3.3	-1.6	3.7	1.8	-1.8	-0.3	3.0	0.1
-0.1	0.8	-0.3	-0.1	0.1	0.6	-7.1	-1.0	-4.3	-6.6	2.1	-10.5	-9.5	5.5	-1.0	-0.2	-0.3	0.1	2.3	0.3	-3.3	-3.0	-2.5	-4.5
dodecane 3		2.2	1.1	2.5	6.0	7.6	8.3	0.7	6.2	4.1	-1.8	1.4	-0.2	2.3	3.6	5.5	8.5	9.2	9.3	7.9	8.7	5.1	1.7
9.2	9.9	8.7	9.2	3.3	1.1	1.4	2.5	5.8	8.8	7.5	1.6	-1.5	2.6	0.1	2.6	2.1	2.0	2.3	0.2	0.0	2.9	6.5	-0.2
6.7	11.5	-0.8	6.5	4.3	-0.1	6.2	5.7	-1.1	0.7	2.6	-0.6	1.5	3.9	-0.2	5.3	6.1	-0.2	3.0	2.2	1.0	1.0	3.3	-2.0
2.4	1.1	-1.4	-0.3	-0.9	1.2	-7.5	3.8	-1.3	-3.8	2.4	-8.9	-8.0	1.9	-0.2	2.8	1.8	0.8	4.1	4.4	-3.6	-2.8	-0.4	-3.0
dodecane 2		1.0	3.6	2.1	5.6	7.5	6.5	-0.1	3.5	5.7	0.9	2.0	1.1	-0.5	2.2	5.2	8.8	9.5	6.3	9.5	11.3	6.8	2.6
9.3	9.3	5.5	6.3	4.3	1.1	-0.5	1.3	1.7	6.7	4.1	1.6	-0.7	4.0	-0.2	2.8	3.1	1.0	1.1	0.9	0.5	-1.5	0.4	0.3
2.6	6.1	0.7	0.4	-0.2	0.7	0.7	8.1	-1.6	0.4	2.2	0.2	0.8	1.8	-1.8	1.6	1.4	0.1	-0.1	1.2	-0.4	0.8	3.2	0.4
0.1	-2.3	-2.6	1.6	1.3	-1.5	-6.0	2.6	-3.8	-4.1	2.9	-11.0	-9.1	2.1	0.3	-0.7	0.4	-0.8	2.7	3.1	-3.4	-3.7	0.4	-3.3
-4.0	-1.5	-0.8	-1.2	3.8	0.9	0.1	1.2	4.3	-0.8	-0.4	0.7	1.0	-0.2										
Avg dodecane		0.7	1.9	1.4	4.5	7.2	6.1	0.0	4.1	4.1	-1.1	0.9	0.9	3.9	5.9	7.5	6.8	9.3	7.5	8.6	10.0	5.1	
1.9	9.3	10.1	6.7	7.4	3.5	0.9	0.8	1.8	3.5	8.0	5.2	0.6	-1.3	4.2	0.5	3.3	1.1	0.8	2.2	0.9	0.2	0.9	3.8
0.5	4.4	8.7	0.3	2.9	1.7	0.2	2.6	7.1	-0.9	0.7	3.1	0.2	0.8	5.2	-1.2	4.9	3.6	-0.6	2.2	1.8	-0.4	0.0	3.2
-0.5	0.8	-0.1	-1.2	0.4	0.2	0.1	-6.9	1.8	-3.1	-4.9	2.5	-10.2	-8.9	3.2	-0.3	0.6	0.6	0.0	3.1	2.6	-3.4	-3.2	-0.8
-3.6	-4.5	0.0	-0.9	-1.1	2.5	0.5	-0.3	0.0	7.0	0.3	-1.9	0.1	2.0	0.6									
octane 1		-4.4	-3.0	-3.6	1.2	6.8	5.0	-3.5	-0.4	-5.1	-5.1	1.8	-1.8	5.8	12.2	11.6	7.8	7.4	11.7	11.0	10.7	9.0	-1.3
9.6	8.8	5.3	4.9	3.3	1.4	-0.2	3.6	5.6	7.1	2.5	5.8	4.9	22.2	0.0	2.7	2.9	1.8	1.7	1.9	0.0	-1.5	3.4	-0.2
0.7	10.1	1.1	0.6	5.6	-0.2	-0.3	7.1	-0.1	1.5	2.3	0.4	1.4	6.7	1.5	3.7	5.5	-0.3	-0.8	0.6	-0.1	0.6	-3.3	0.6
0.8	-2.1	1.9	1.0	0.8	-0.1	1.0	2.3	1.0	0.8	5.0	-1.0	0.5	4.4	1.8	-1.0	4.5	0.1	2.6	1.4	-1.6	3.0	0.8	3.7
3.1	4.7	1.4	6.9	9.3	0.9	5.7	5.1	10.0	11.7	7.5	0.0	8.5	10.0										
octane 2		1.0	1.5	3.0	5.2	12.3	10.8	-1.4	6.3	5.5	-2.4	3.3	5.3	11.9	17.0	17.7	10.0	13.5	12.5	9.1	10.2	9.0	4.9
10.4	14.5	5.7	9.1	8.8	1.5	0.5	1.5	7.6	7.2	5.6	5.9	8.2	23.9	0.4	2.7	1.5	1.2	1.2	-1.2	-0.3	1.8	4.2	0.4
3.2	10.8	0.3	1.2	3.0	0.4	1.6	4.0	-1.3	-0.1	0.3	0.5	0.0	4.4	-0.5	3.0	3.1	0.4	-0.4	2.5	1.1	1.5	-0.5	-0.3
0.7	0.0	-2.6	-0.4	0.6	-2.2	-4.4	1.0	-2.8	-0.9	1.5	-2.5	-2.1	4.2	-0.4	0.7	1.7	-1.2	2.5	1.8	-0.2	1.4	3.9	-2.2
1.1	1.4	-0.8	4.3	2.5	0.8	2.7	7.9	6.8	6.2	3.4	-0.5	4.3	4.7										
octane 3		-2.3	0.9	-1.3	3.2	10.4	11.8	-2.1	0.9	-0.4	-5.2	-3.2	-3.0	10.8	17.8	12.1	14.1	13.5	15.3	13.1	13		

-0.4	2.5	3.4	0.1	0.7	0.8	1.2	0.7	4.4	0.5	0.7	5.2	0.5	1.3	4.2	-0.8	4.6	2.3	0.2	3.5	0.6	-0.5	0.0	4.2	
-0.4	1.0	1.1	-0.1	0.6	0.3	-0.2	-6.4	0.8	-4.7	-5.3	4.2	-11.3	-10.1	4.0	-0.6	0.1	-2.6	1.7	1.9	5.0	-4.3	-4.7	0.7	
-5.1	-4.9	-1.1	0.4	-1.2	0.7	1.3	0.2	2.2	10.9	0.6	1.5	-0.3	4.0	1.7										
tetradecane 3	0.4	0.8	0.5	1.1	2.9	3.2	0.1	3.0	3.8	-1.1	-0.3	1.8	5.3	4.9	4.2	4.9	6.3	5.3	4.8	4.8	3.4			
	1.8	5.0	7.2	4.2	4.5	1.3	1.5	1.3	1.1	4.8	3.0	2.6	0.4	4.8	-0.1	2.1	1.5	-0.3	2.9	-0.4	-0.2	1.3	3.5	
	-0.9	0.7	3.3	0.6	0.5	0.4	-0.1	3.0	4.6	-3.5	-2.2	2.2	0.4	0.8	2.1	0.5	5.5	3.6	0.2	3.1	2.3	0.6	0.5	1.1
	0.6	0.5	2.1	1.7	0.4	0.7	-0.4	4.1	2.5	-2.0	-1.8	1.2	-7.3	-7.5	5.6	-0.8	0.0	-0.8	-0.9	3.5	2.8	-1.0	-3.4	0.5
	-1.2	-2.0	2.1	0.8	1.0	1.9	0.0	1.2	3.7	7.1	1.0	0.0	0.0	4.2	3.9									
Avg tetradecane	-0.6	0.8	0.6	0.6	3.4	1.4	0.0	2.8	3.0	-0.3	1.0	2.8	3.5	5.3	4.5	5.6	5.2	6.0	4.8	4.9	2.6			
	0.8	5.7	5.3	3.5	3.8	2.2	0.6	0.5	0.8	0.4	4.1	3.5	1.5	1.8	3.2	0.2	2.4	1.4	-0.2	2.3	1.0	-0.1	0.6	3.5
	-0.2	1.1	3.2	-0.2	0.8	1.1	0.5	1.4	5.5	-1.1	-0.2	4.1	0.5	1.2	4.1	-0.1	4.7	4.0	0.3	2.7	2.1	-0.4	-0.1	2.6
	0.2	0.3	1.2	-0.6	0.4	0.3	0.0	-5.1	0.8	-3.1	-2.7	3.1	-8.5	-8.2	3.3	-0.5	0.6	-1.2	0.4	1.7	3.5	-2.7	-3.1	-0.2
	-2.6	-2.7	-0.3	0.5	0.1	2.0	0.4	0.6	3.2	8.5	0.4	1.2	-0.1	3.4	2.1									
1-octene 1	-0.4	0.4	-0.1	7.6	10.2	11.4	-3.0	25.6	2.1	3.7	20.0	12.6	7.7	13.2	14.0	7.7	10.7	8.8	13.4	14.4	12.3	0.1		
	6.2	8.6	5.2	5.3	6.4	3.1	-0.5	3.1	11.0	10.2	3.9	9.3	11.4	33.5	0.6	0.3	-0.6	-1.4	1.3	1.5	-0.3	-0.1	1.1	-0.4
	1.2	1.9	-0.5	-0.1	1.8	-0.3	0.8	0.9	0.2	1.0	2.3	-0.2	3.3	3.1	0.2	3.9	3.5	-0.6	2.2	2.3	0.5	0.6	2.3	0.8
	2.4	1.6	-1.0	-0.5	0.2	0.3	-4.8	3.8	-0.5	-0.6	1.9	-6.4	-5.8	5.3	-1.4	0.7	2.4	-0.4	0.4	4.8	-2.4	-2.9	-0.3	3.9
	3.8	4.9	-0.6	2.1	0.5	1.2	2.0	2.4	-3.0	-0.8	-2.3	0.0	2.8	7.8										
1-octene 2	-0.1	0.2	0.9	5.1	6.8	7.7	-4.2	16.3	0.2	2.1	8.5	7.1	3.4	7.6	8.8	5.5	6.8	7.3	9.2	9.6	8.9	0.7		
	5.9	7.7	3.6	5.4	3.9	1.2	-0.9	1.8	7.7	8.3	4.4	9.1	9.9	28.8	-0.1	2.2	2.5	1.4	1.5	1.1	0.2	0.8	3.5	0.1
	3.1	3.1	0.3	2.7	0.7	-0.2	1.9	3.4	0.3	1.6	3.5	0.3	0.4	2.2	0.5	4.0	4.0	0.8	3.1	2.8	2.0	1.5	4.1	2.2
	2.4	0.3	-1.6	0.7	0.1	-1.0	-5.1	2.0	-1.6	-0.3	2.2	-7.2	-5.8	5.0	-0.2	0.5	2.1	-0.2	2.0	5.9	-1.6	-2.0	-1.4	6.5
	3.6	3.5	0.3	1.3	1.8	0.2	2.7	-0.2	0.7	2.0	1.6	-0.5	5.2	6.8										
1-octene 3	-0.6	1.7	1.5	8.4	7.6	11.7	-1.8	24.2	2.7	2.5	10.5	12.1	7.6	14.8	13.5	8.9	10.8	10.3	10.8	10.4	12.3	1.0		
	4.7	8.3	4.1	4.8	6.8	0.8	-2.0	3.1	6.6	6.1	3.4	10.0	11.4	31.4	0.2	1.9	-2.1	0.1	1.3	0.9	0.1	0.2	1.8	-0.2
	1.9	0.2	0.3	1.9	-1.4	0.7	1.3	1.1	0.3	1.7	0.4	0.0	0.4	0.0	-0.1	2.9	2.7	-1.0	4.8	0.7	-0.4	0.1	2.1	0.3
	1.3	-0.5	-0.8	-1.0	-0.8	1.0	-5.7	2.1	-0.8	-4.5	1.5	-6.6	-6.6	2.8	0.2	-0.5	0.1	-1.6	0.5	0.9	-2.2	-2.5	-0.4	6.9
	4.4	8.0	-0.1	-0.8	0.2	0.8	1.5	1.7	1.5	0.9	-1.3	0.2	2.8	4.8										
Avg 1-octene	-0.4	0.8	0.8	7.0	8.2	10.3	-3.0	22.0	1.7	2.8	13.0	10.6	6.2	11.9	12.1	7.3	9.4	8.8	11.1	11.5	11.2			
	0.6	5.6	8.2	4.3	5.2	5.7	1.7	-1.1	2.7	8.4	8.2	3.9	9.5	10.9	31.2	0.2	1.5	-0.1	0.0	1.4	1.2	0.0	0.3	2.1
	-0.2	2.1	1.7	0.1	1.5	0.4	0.1	1.4	1.8	0.3	1.4	2.1	0.0	1.4	1.8	0.2	3.6	3.4	-0.3	3.4	1.9	0.7	0.8	2.8
	1.1	2.0	0.5	-1.1	-0.3	-0.2	0.1	-5.2	2.6	-1.0	-1.8	1.9	-6.7	-6.0	4.4	-0.5	0.2	1.5	-0.7	1.0	3.8	-2.1	-2.4	-0.7
	5.7	3.9	5.5	-0.1	0.9	0.8	0.7	2.1	1.3	-0.3	0.7	-0.6	-0.1	3.6	6.5									
trans-5-decene 3	0.0	1.6	1.3	5.1	5.7	13.4	-11.7	13.6	-2.9	-4.2	27.3	6.4	5.8	11.0	12.6	5.6	7.7	9.6	14.0	13.0	13.1			
	-5.0	2.6	5.5	-0.3	0.1	1.8	4.8	0.4	2.6	4.5	3.9	1.0	3.3	9.0	25.2	0.1	0.9	-2.9	-5.1	0.7	-4.2	-3.1	-6.1	-1.8
	-6.1	-2.2	-0.7	-1.1	1.8	1.3	1.0	1.9	1.7	-0.8	-0.9	2.4	-0.1	-0.7	0.0	-0.7	6.7	4.3	0.7	4.0	1.5	6.8	6.2	8.3
	8.3	7.9	11.0	3.8	4.0	5.5	1.7	-0.3	5.7	6.5	3.9	4.1	-0.9	-1.7	8.4	-0.5	9.7	5.2	3.0	3.3	2.0	1.7	1.1	1.3
	29.0	21.0	9.9	0.5	8.2	8.3	11.3	13.3	10.5	8.0	4.0	0.6	0.0	9.9	13.4									
trans-5-decene 2	-4.7	-3.3	-3.1	5.9	6.9	15.9	-12.0	14.1	-3.9	-2.1	30.0	7.7	8.1	13.9	12.9	13.6	15.0	14.3	12.2	12.7	11.9			
	0.1	7.4	12.0	7.6	7.1	10.3	0.0	-0.6	1.4	5.6	7.0	4.5	7.8	13.0	28.0	-0.6	3.8	1.2	5.1	4.6	6.1	0.7	4.7	6.2
	-1.1	7.7	4.3	-0.5	3.5	1.3	-0.3	0.1	-1.5	2.3	2.1	1.3	2.1	1.9	-0.6	4.3	-1.2	0.0	1.9	1.8	3.5	2.0	2.9	
	-0.3	-0.3	0.2	2.0	2.3	1.9	0.2	-3.7	0.8	-3.7	-4.1	-0.9	-3.6	-4.5	6.7	0.4	4.7	3.7	0.1	1.4	2.9	-6.9	-5.3	-3.2
	16.7	9.1	3.5	-4.7	-5.2	-5.2	4.9	3.8	2.0	5.7	3.7	-1.0	0.4	5.8	10.2									
trans-5-decene1	-5.3	-3.6	-3.6	3.2	6.7	12.8	-12.2	13.1	-3.6	-3.0	27.9	6.7	6.1	12.4	14.2	9.7	11.2	11.2	12.3	12.3	12.3			
	-4.1	4.9	8.8	2.9	2.5	5.5	1.4	-1.5	2.2	5.2	5.6	3.2	5.4	8.2	22.1	-0.3	2.4	-0.8	-0.1	2.3	0.5	-1.0	1.7	1.9
	-2.4	2.7	1.1	-0.6	3.2	1.5	0.4	1.5	-1.3	1.6	1.1	2.8	0.6	0.8	1.7	-0.4	5.3	2.7	0.2	-1.9	0.7	6.6	5.7	-0.2
	2.9	3.3	0.4	5.3	4.5	3.7	0.9	0.9	9.2	3.2	4.6	9.4	0.2	11.8	12.3	2.1	-0.2	7.2	4.6	0.8	-0.5	0.7	3.1	5.0
	32.7	20.8	8.4	-1.7	4.3	4.0	9.6	9.3	6.3	6.2	3.8	0.3	0.6	7.4	11.6									
trans-5-deceneAvg	-3.3	-1.8	-1.8	4.7	6.4	14.0	-12.0	13.6	-3.4	-3.1	28.4	6.9	6.7	12.4	13.2	9.6	11.3	11.7	12.8	12.6				
	12.4	-3.0	5.0	8.7	3.4	3.2	5.9	2.1	-0.6	2.1	5.1	5.5	2.9	5.5	10.1	25.1	-0.3	2.4	-0.8	0.0	2.5	0.8	-1.1	-1.0
	2.1	-3.2	2.7	1.6	-0.7	2.8	1.4	0.4	1.2	-0.4	1.1	0.8	2.2	0.9	0.7	1.2	-0.5	5.4	2.0	0.3	1.3	1.3	5.6	4.6
	3.6	3.6	3.6	3.9	3.7	3.6	3.7	0.9	1.7	3.2	2.5	3.1	1.1	2.4	2.0	5.7	-0.1	7.2	4.5	1.3	1.4	-0.7	0.3	
	0.5	26.1	16.9	7.2	-2.0	2.4	2.4	8.6	8.8	6.3	6.7	3.8	0.0	0.3	7.7	11.7								
cyclohexene 1	0.9	-2.8	-1.5	6.3	9.2	12.9	0.5	1.0	2.6	1.1	8.6	12.0	6.2	12.9	11.9	7.1	9.2	6.2	13.7	12.4	10.1			
	1.6	6.7	8.0	5.9	13.2	-0.7	-1.6	-1.1	9.5	10.0	4.7	-2.2	-7.2	-5.7	0.4	1.2	-5.3	1.6	3.2	-0.7	0.0	0.6	-0.5	
	0.0	5.4	0.4	0.1	0.6	-0.2	1.3	-1.9</																

27.0	1.0	-0.3	4.1	-8.7	0.4	5.2	-4.4	-1.3	13.6	-22.6	-17.3	16.9	-10.3	-41.3	11.8	-38.1	-40.4	44.8	-37.1	-28.1	38.0	-2.1	-8.5
11.1	-0.4	19.0	17.0	-15.8	-9.6	-5.3	-5.9	1.3	-3.5	-0.5	-6.4	4.4	-1.8	-2.2	2.6	1.0	1.3	1.9	0.2	4.1	-1.1		
benzylamine	2	2.7	-24.0	20.7	-41.8	26.1	-9.9	-45.7	12.8	-24.1	-11.9	16.0	-25.7	16.8	7.6	18.9	84.3	5.9	40.7	1.3	-0.8	-9.5	
	-30.9	-1.0	-12.3	-9.5	1.7	-5.5	63.8	-18.8	15.7	48.1	-5.6	10.1	-0.3	-1.0	0.7	-96.9	13.0	-52.7	9.4	95.4	-84.7	-145.0	-99.8
77.4	-177.0	-90.3	55.5	-190.0	-	-93.7	77.6	-150.5	-	-121.5	-	49.5	-143.5	-	-87.3	92.4	-200.6	-	-103.8	-	113.1	-0.4	
90.9	37.1	1.1	3.0	11.7	-6.2	4.2	4.8	-3.2	-1.1	11.9	-23.2	-18.5	17.2	-6.0	-39.9	10.8	-29.4	-35.8	46.1	-30.7	-22.9	36.8	0.2
-5.3	12.4	-2.0	20.7	21.1	-16.5	-15.3	-10.9	-9.3	-3.9	-6.0	-0.3	-7.1	1.2	0.9	-3.4	5.2	0.4	4.6	3.3	-0.6	1.8	-2.4	
Avg benzylamine	4.1	-22.9	23.7	-40.0	28.3	-8.3	-43.2	19.1	-19.7	-6.5	20.1	-20.7	13.8	2.4	13.6	83.6	2.1	36.5	2.5	-0.4	-9.1		
	-26.1	1.4	-11.3	-5.9	4.3	-2.4	64.8	-18.9	13.6	55.6	-5.4	14.1	1.0	1.4	2.0	-97.2	9.9	-50.0	6.7	92.2	-81.9	-141.1	-96.8
79.1	-176.5	-90.6	58.5	-191.7	-	-95.6	74.5	-145.4	-	-119.3	-	63.5	-141.9	-	-86.0	95.1	-197.0	-	-101.7	-	114.1	-0.3	
88.6	32.1	1.1	1.3	7.9	-7.5	2.3	5.0	-3.8	-1.2	12.8	-22.9	-17.9	17.0	-8.2	-40.6	11.3	-33.8	-38.1	45.4	-33.9	-25.5	37.4	-0.9
-6.9	11.8	-1.2	19.8	19.0	-16.1	-12.4	-8.1	-7.6	-1.3	-4.7	-0.4	-6.7	2.8	-0.4	-2.8	3.9	0.7	2.9	2.6	-0.2	3.0	-1.8	
2-ethyl-1-hexylamine	1	5.4	-3.2	32.3	-17.8	39.0	9.2	-20.5	25.8	-12.1	2.8	28.6	-8.6	75.1	0.0	25.2	93.6	9.4	42.9	21.1	13.4		
	-8.7	-14.4	10.2	5.8	-1.9	11.0	5.1	50.9	-23.0	16.3	64.6	-5.8	24.6	3.2	2.4	-0.3	-55.7	29.9	-42.6	29.4	103.9	-39.5	-96.8
53.2	-139.9	-82.1	62.8	-172.1	-	-83.8	97.3	-102.7	-	-99.3	37.0	-100.1	-	-81.1	75.0	-178.6	-	-101.6	-	109.6	-0.2	90.7	
37.6	-0.5	4.0	30.4	13.7	8.8	-6.5	18.5	4.5	3.9	-16.0	-14.6	16.5	-7.0	-24.5	9.7	-20.6	-30.0	27.2	-18.9	-21.1	25.4	0.0	-7.5
12.9	0.4	39.2	46.8	-25.2	-18.1	-20.7	18.7	18.2	0.2	-15.8	-19.7	0.9	-7.0	-11.7	2.3	6.5	-6.0	-21.1	-4.1	-13.0	-27.0		
2-ethyl-1-hexylamine	2	2.6	-7.8	30.6	-18.1	40.1	7.5	-20.3	27.4	-12.5	3.5	38.2	-5.1	82.2	6.5	37.9	106.2	15.1	50.6	20.2	13.6		
	-6.9	-9.7	11.6	8.9	-2.5	11.5	4.3	46.6	-19.9	7.6	66.3	-3.6	29.9	4.3	7.9	5.9	-65.9	35.4	-42.4	39.0	108.8	-41.8	-107.4
-82.4	59.8	-152.7	-	-83.6	55.0	-183.9	-	-88.7	96.6	-118.2	-	-108.0	-	34.3	-106.3	-	-79.2	89.2	-188.2	-	-104.4	-	107.1
0.9	88.4	42.6	0.3	2.6	31.6	12.9	8.4	-4.5	19.0	5.5	2.5	-25.3	-24.6	22.0	-9.4	-20.4	12.4	-19.5	-25.4	27.2	-14.4	-17.0	23.8
-0.1	-8.1	15.8	1.5	40.0	46.0	-23.9	-18.4	-20.6	22.0	15.7	1.9	-16.1	-20.7	1.8	-2.3	-12.4	0.2	7.4	-0.8	-16.4	-3.2	-6.7	-22.1
2-ethyl-1-hexylamine	3	6.4	-6.6	32.4	-16.4	38.7	10.1	-15.5	34.2	-5.4	4.3	40.4	-6.1	78.8	8.5	36.3	92.4	16.3	49.5	25.5	18.9		
	-0.9	-13.0	9.4	4.9	1.9	13.4	5.7	54.1	-20.7	17.7	60.7	-5.9	20.4	7.9	8.0	5.1	-67.9	28.0	-40.9	32.7	105.1	-41.6	-105.0
-80.2	51.0	-149.0	-	-82.0	52.3	-178.4	-	-85.2	91.1	-111.4	-	-106.2	-	25.8	-105.6	-	-78.3	74.4	-186.8	-	-105.3	-	103.8
0.8	87.0	41.6	-0.6	3.5	30.4	15.5	6.9	-6.1	21.1	5.3	1.7	-15.8	-15.0	16.2	-2.9	-19.9	9.7	-23.3	-47.7	36.9	-13.4	-16.6	24.4
0.7	-2.8	17.0	-0.1	41.7	43.6	-15.7	-13.0	-11.3	24.2	20.2	8.6	-11.1	-11.3	6.9	5.0	-1.1	9.9	8.8	4.8	-10.3	0.2	-9.4	-25.3
Avg 2-ethyl-1-hexylamine	4.8	-5.9	31.7	-17.4	39.3	8.9	-18.8	29.2	-	-10.0	3.5	35.8	-6.6	78.7	5.0	33.1	97.4	13.6	47.7	22.2			
	15.3	-5.5	-12.3	10.4	6.6	-0.8	12.0	5.0	50.5	-21.2	13.9	63.8	-5.1	25.0	5.1	6.1	3.6	-63.1	31.1	-42.0	33.7	105.9	-40.9
103.0	-79.8	54.7	-147.2	-	-82.6	56.7	-178.1	-	-85.9	95.0	-110.8	-	-104.5	-	32.4	-104.0	-	-79.5	79.5	-184.6	-	-103.8	
106.8	0.5	88.7	40.6	-0.3	3.4	30.8	14.0	8.0	-5.7	19.5	5.1	2.7	-19.0	-18.1	18.2	-6.4	-21.6	10.6	-21.1	-34.3	30.4	-15.6	-18.3
24.5	0.2	-6.1	15.2	0.6	40.3	45.5	-21.6	-16.5	-17.5	21.6	18.0	3.6	-14.3	-17.2	3.2	-1.4	-8.4	4.1	7.6	-0.7	-15.9	-2.4	-9.7
-24.8																							
2-heptylamine	1	1.1	-8.6	19.9	-14.8	32.2	4.7	-18.4	23.1	-13.3	1.2	30.1	-13.0	23.3	8.7	23.9	57.3	11.1	46.3	20.2	11.7	5.2	
	-12.4	5.1	7.8	-0.5	8.5	6.6	40.9	-35.0	24.1	67.4	2.6	35.9	2.5	10.3	12.4	-78.9	21.7	-36.0	16.8	93.6	-46.8	-119.8	-89.8
68.1	-147.7	-	-81.7	70.6	-178.8	-	-81.0	103.6	-118.2	-	-104.2	-	52.2	-111.3	-	-80.2	87.9	-178.5	-	-93.5	120.7	0.7	86.1
44.8	0.1	4.0	33.4	12.1	12.1	-1.5	13.1	5.7	2.7	-19.3	-10.6	21.3	-6.8	-13.6	15.9	-17.9	-20.7	39.0	-7.5	-5.6	36.3	0.2	0.1
23.6	0.6	37.7	47.1	-26.9	-21.7	-18.9	14.3	5.1	-6.2	-12.8	-17.9	4.9	-4.5	-2.9	-0.8	0.3	3.5	-11.4	0.0	-10.5	-30.7		
2-heptylamine	2	5.9	-5.8	23.7	-14.9	33.4	8.9	-20.7	26.9	-14.2	-0.7	32.3	-13.3	17.8	7.7	19.0	66.9	12.2	49.0	19.4	11.9	2.5	
	-10.9	6.2	6.9	-0.6	8.6	7.6	39.5	-36.2	17.9	62.2	0.5	34.1	3.0	6.4	12.7	-80.5	20.0	-34.4	20.0	97.3	-38.0	-123.8	-94.1
71.6	-148.7	-	-78.8	67.9	-181.6	-	-83.0	99.1	-116.2	-	-103.0	-	48.7	-118.9	-	-84.7	85.8	-185.9	-	-97.1	118.1	0.2	87.1
48.2	-1.2	3.3	35.0	10.8	10.6	-0.8	16.2	4.0	6.5	-20.1	-14.7	17.6	-3.6	-17.3	13.2	-17.9	-23.5	31.9	-9.7	-7.2	32.7	0.8	4.1
20.7	-0.5	38.6	53.6	-19.5	-16.1	-14.4	14.0	4.9	-6.3	-15.8	-17.9	2.2	-11.4	-0.8	6.1	2.2	4.0	-9.6	0.3	-10.0	-26.8		
2-heptylamine	3	0.5	-12.5	22.0	-12.7	31.8	7.5	-25.5	22.3	-14.9	2.5	31.0	-3.5	17.2	6.9	20.0	70.0	11.0	47.8	18.8	11.4	1.2	
	-11.4	4.2	4.9	-0.7	7.8	5.6	33.2	-36.4	8.4	55.0	-3.9	25.3	-1.7	6.6	7.0	-77.4	16.5	-42.9	18.7	83.2	-50.2	-122.8	-95.2
56.2	-154.7	-	-85.0	55.4	-181.4	-	-84.6	91.8	-121.4	-	-111.7	-	30.3	-121.2	-	-91.7	79.4	-188.6	-	-105.2	-	107.3	1.0
81.2	45.4	-1.3	3.6	30.2	6.1	3.4	3.1	7.2	-2.6	-0.6	-26.3	-19.7	15.3	-6.0	-23.7	6.0	-19.6	-30.6	22.8	-17.7	-16.5	18.7	0.9
-9.6	9.6	-0.1	30.8	38.4	-18.0	-13.6	-13.7	14.4	6.6	-5.7	-11.4	-17.9	-0.2	-7.7	-4.2	2.4	-0.9	-2.9	-11.5	0.2	-8.5	-18.8	
Avg 2-heptylamine	2.5	-9.0	21.8	-14.1	32.4	7.0	-21.5	24.1	-14.1	1.0	31.1	-10.0	19.4	7.8	21.0	64.7	11.4	47.7	19.5	11.7			
	3.0	-11.6	5.2	6.6	-0.6	8.3	6.6	37.8	-35.9	16.8	61.5	-0.3	31.8	1.3	7.8	10.7	-78.9	19.4	-37.8	18.5	91.4	-45.0	-122.1
-93.0	65.3	-150.4	-	-81.8	64.6	-180.6	-	-82.9	98.2	-118.6	-	-106.3	-	43.7	-117.1	-	-85.5	84.4	-184.4	-	-98.6	115.4	0.6
84.8	46.1	-0.8	3.6	32.8	9.7	8.7	-1.8	12.2	2.4	2.9	-21.9	-15.0	18.1	-5.5	-18.2	11.7	-18.5	-24.9	31.2	-11.6	-9.8	29.2	0.6
-1.8	18.0	0.0	35.7	46.4	-21.5	-17.1	-15.7	14.2	5.5	-6.1	-13.3	-17.9	2.3	-7.9	-2.6	2.6	0.5	1.5	-10.8	0.1	-9.7	-25.4	
3,5-dimethylaniline	3	-15.9	-17																				

83.1	33.8	-0.2	-0.3	24.4	5.9	6.9	-0.6	7.8	1.7	9.6	-28.7	-22.9	14.8	-15.7	-48.6	9.9	-40.4	-53.4	47.1	-43.8	-38.7	61.0	0.7
-8.5	4.8	0.4	34.9	43.5	-27.5	-32.0	-24.8	15.8	-0.6	-7.8	-12.6	-15.6	-11.0	-3.1	4.2	8.1	4.9	-4.7	-15.2	-0.7	-9.5	-17.0	
amylamine 2			3.8	-8.2	23.2	-14.9	31.0	1.9	-14.1	15.5	-12.9	-3.3	20.2	-23.8	51.8	-3.4	33.1	68.4	-2.1	35.6	19.1	7.9	-8.1
-16.7	1.7	0.5	-7.9	4.7	-6.1	55.4	-23.5	21.8	61.8	-1.9	24.7	-0.3	-2.4	-4.1	-107.3	-2.6	-12.6	-36.5	58.5	-39.0	-124.1		
-85.7	69.0	-162.9		-77.5	75.1	-179.1		-82.6	103.4	-121.0		-104.6		50.9	-124.8		-84.6	74.0	-192.8		-97.6	107.9	-5.5
76.2	33.3	-5.6	-3.7	18.7	0.9	2.2	-1.8	3.8	-2.5	7.5	-36.7	-27.4	3.1	-25.5	-54.6	2.2	-46.7	-58.7	35.9	-46.2	-41.1	50.5	-4.0
-13.3	5.1	-10.4	29.7	44.4	-38.0	-39.2	-34.1	8.4	-8.3	-15.5	-25.0	-24.6	-14.8	-8.5	0.8	2.0	9.1	-4.6	-18.2	-9.4	-14.6	-18.4	
amylamine 3			2.0	-16.0	20.9	-21.6	28.4	-3.1	-8.0	12.8	-10.6	0.2	13.1	-17.6	51.1	-7.0	29.2	68.8	-3.0	35.7	9.9	3.5	-11.0
-17.7	3.1	-2.3	-7.1	5.6	-4.1	62.7	-19.4	19.4	64.3	-9.4	18.1	0.7	1.5	3.6	-103.6	-5.5	-15.6	-39.9	55.8	-42.6	-128.4		
-90.5	65.9	-163.7		-81.6	71.5	-178.6		-83.9	97.9	-125.5		-110.2		48.5	-132.9		-87.3	85.1	-193.5		-104.5	108.1	
-0.4	84.0	32.3	0.4	1.5	14.3	-1.8	-1.1	2.4	-2.9	-7.0	7.9	-29.9	-25.7	10.7	-16.2	-54.7	6.7	-41.8	-60.2	47.5	-47.6	-48.5	58.5
0.2	-10.5	1.9	-1.9	24.7	36.2	-26.8	-31.3	-27.1	-4.1	-15.5	-15.2	-6.3	-13.1	-9.7	-0.6	-8.8	-1.5	-0.7	-2.8	-8.7	0.4	3.9	-0.3
Avg amylamine			2.1	-9.7	19.6	-16.2	31.0	0.3	-8.9	17.1	-8.6	-0.3	20.5	-19.0	55.7	-2.4	32.7	70.4	0.0	37.0	13.9	4.3	-12.2
-15.3	3.7	1.2	-6.9	7.0	-4.4	58.0	-20.8	21.8	63.1	-2.3	24.1	1.4	-0.2	-0.1	-103.8	-2.5	-12.1	-37.8	58.1	-39.3	-124.2		
-86.2	68.8	-163.5		-80.1	74.0	-175.8		-82.1	102.3	-120.8		-105.4		51.1	-127.0		-84.3	81.9	-191.4		-97.9	110.6	-1.7
81.1	33.1	-1.8	-0.8	19.1	1.7	2.7	0.0	2.9	-2.6	8.3	-31.8	-25.3	9.6	-19.2	-52.6	6.3	-43.0	-57.5	43.5	-45.8	-42.7	56.7	-1.0
-10.8	3.9	-4.0	29.8	41.4	-30.7	-34.2	-28.7	6.7	-8.2	-12.8	-14.6	-17.7	-11.8	-4.1	-1.3	2.9	4.4	-4.0	-14.0	-3.2	-6.7	-11.9	
cyclooctylamine 1			-15.5	-29.6	5.4	-42.9	16.0	-9.9	-32.4	8.1	-14.5	-20.6	1.7	-25.8	4.7	-19.0	9.8	63.7	-7.3	27.6	6.7	0.1	-11.4
-42.9	-1.6	-14.0	-15.9	-3.6	-13.9	64.2	-29.5	5.0	33.7	-10.9	4.2	-3.2	0.0	3.4	-120.3		-13.9	-41.4	-35.4	60.7	-69.3	-143.4	
-99.4	69.9	-178.6		-101.8		54.8	-191.5		-95.5	93.7	-143.4		-122.8		49.4	-151.8		-110.4		78.8	-199.5		
114.0	103.0	-0.9	74.7	29.7	-1.5	-6.9	12.9	-20.8	-15.0	-8.9	-14.7	-15.1	-0.7	-42.9	-31.8	-1.1	-24.0	-57.5	2.6	-53.5	-61.6	35.7	-49.0
-38.4	47.6	-6.3	-25.4	1.1	-6.8	25.3	29.8	-25.6	-19.3	-13.5	-1.3	4.7	-6.4	-5.1	-13.8	-0.6	-10.3	-8.6	4.5	4.2	-1.9	-2.2	1.8
-2.4	-17.4																						
cyclooctylamine 2			-5.1	-29.8	12.7	-41.2	22.1	-6.4	-28.5	0.1	-24.2	-23.9	-2.7	-29.3	11.5	-16.6	12.4	69.4	-7.3	32.9	5.2	0.4	-9.1
-31.2	0.3	-10.0	-14.1	-1.2	-12.7	64.9	-29.7	8.6	51.3	-8.6	10.5	-2.2	-0.9	2.2	-116.4		-10.7	-32.9	-27.3	69.2	-66.2	-144.0	
-101.0	73.4	-179.5		-98.9	55.4	-201.1		-97.7	95.7	-155.7		-132.2		41.1	-154.9		-105.2		92.4	-210.0			
119.3	100.6	-0.3	79.8	29.3	-16.7	-20.6	8.1	-24.9	-20.0	-11.4	-23.2	-26.3	-4.0	-41.1	-31.4	5.1	-20.3	-61.3	-2.1	-53.6	-64.2	23.8	-51.5
-42.5	45.0	0.0	-29.3	-4.4	-3.5	27.7	31.2	-38.4	-32.0	-24.7	-0.9	1.4	-9.6	-13.2	-24.6	-5.6	-3.9	2.3	2.9	4.1	-6.1	-5.4	6.2
-19.3	-37.5																						
cyclooctylamine 3			-29.4	-49.3	-5.1	-52.7	8.0	-16.7	-41.6	-13.2	-35.4	-31.1	-1.4	-36.1	1.7	-22.3	8.1	57.3	-11.2	24.1	1.2	-5.3	-14.8
-40.3	-7.6	-18.1	-22.9	-10.7	-21.5	57.9	-31.9	1.9	35.3	-22.7	-5.6	-12.1	-6.5	-4.7	-117.5		-8.6	-38.2	-29.2	68.9	-71.7	-146.9	
-105.2	71.2	-182.2		-102.6		50.0	-198.9		-100.3		89.1	-156.4		-136.1		33.8	-149.1		-103.4		85.9		
206.2	-118.4		101.6	-0.1	76.4	27.8	-2.1	-8.5	10.1	-25.2	-21.6	-12.1	-20.6	-25.4	-5.0	-42.2	-29.5	3.8	-20.6	-62.7	-2.0	-58.0	-67.0
24.8	-53.0	-44.4	43.8	0.0	-25.9	-1.3	-3.6	29.8	32.5	-32.7	-21.9	-15.2	3.4	7.6	-6.6	-8.0	-25.4	-1.9	-9.3	-4.9	9.9	-0.7	-5.8
-6.0	-0.3	-28.2	-52.1																				
Avg cyclooctylamine			-16.6	-36.2	4.3	-45.6	15.4	-11.0	-34.2	-1.7	-24.7	-25.2	-0.8	-30.4	6.0	-19.3	10.1	63.5	-8.6	28.2	4.4	-1.6	
-11.7	-38.1	-3.0	-14.1	-17.6	-5.1	-16.0	62.4	-30.4	5.1	40.1	-14.1	3.0	-5.9	-2.5	0.3	-118.1		-11.1	-37.5	-30.6	66.2	-69.1	
144.8	-101.9	71.5	-180.1		-101.1		53.4	-197.2		-97.8	92.9	-151.8		-130.4		41.4	-151.9		-106.3		85.7		
205.2	-117.2		101.7	-0.4	76.9	28.9	-6.8	-12.0	10.4	-23.7	-18.9	-10.8	-19.5	-22.3	-3.2	-42.1	-30.9	2.6	-21.6	-60.5	-0.5	-55.0	-64.2
28.1	-51.2	-41.8	45.5	-0.1	-26.8	-1.5	-4.6	27.6	31.2	-32.3	-24.4	-17.8	0.4	4.5	-7.5	-8.7	-21.2	-2.7	-7.8	-3.7	5.7	2.5	-4.6
-4.5	2.6	-16.6	-35.7																				
dipropylamine 1			6.1	-14.8	29.7	-22.0	24.1	1.6	-22.5	1.0	-19.0	-22.7	9.9	-21.0	-24.5	-7.2	-13.9	50.3	-8.3	26.4	19.5	12.6	1.0
-13.8	9.2	-1.0	-1.8	3.1	2.2	43.4	-27.1	12.8	50.9	-13.2	22.1	-11.7	-0.7	7.7	-66.4	31.6	-37.7	49.6	122.0	-44.4	-129.9		
102.0	68.0	-166.8		-94.6	48.1	-190.7		-96.8	94.7	-129.4		-123.7		32.5	-141.0		-106.1		94.1	-194.4		-109.6	
109.9	0.5	88.4	37.5	-0.7	4.0	24.5	5.8	-3.0	-11.6	4.3	-7.3	-7.1	-14.8	-6.4	12.3	-8.1	-36.4	7.9	-15.4	-29.7	19.0	-7.4	-10.2
20.4	-0.4	-7.3	4.4	-0.3	40.1	46.9	-19.3	-15.2	-12.0	-0.3	2.9	-5.6	-1.8	-17.4	7.2	0.7	-2.0	8.1	-0.1	13.7	1.9	-0.2	0.1
-26.9																							
dipropylamine 2			5.5	-12.3	41.3	-22.3	25.4	-0.4	-17.1	7.2	-16.8	-14.8	14.9	-9.9	-19.7	-0.2	-9.5	68.8	2.4	34.6	17.7	9.7	3.8
-18.6	5.6	-3.8	0.7	3.8	3.7	39.2	-25.2	-1.5	61.0	-9.1	22.2	-5.2	6.2	9.0	-76.2	24.4	-34.9	36.8	100.4	-71.7	-131.1		
100.8	57.7	-168.2		-94.1	41.8	-199.5		-99.7	95.2	-135.4		-125.7		28.9	-143.0		-105.8		77.4	-199.2		-112.3	
101.6	-1.3	85.0	38.1	-1.8	1.4	27.2	2.4	-5.8	-11.4	-3.0	-8.6	-3.6	-18.0	-9.2	5.0	-13.4	-33.1	5.4	-17.5	-31.1	17.8	-9.7	-14.4
18.6	0.8	-10.1	5.4	0.5	36.2	40.4	-16.2	-22.8	-26.5	-0.4	-0.4	-8.3	-3.3	-13.7	8.9	-1.6	-2.9	10.7	-0.2	8.6	-2.2	-0.8	-4.2
-23.7																							
dipropylamine 3			5.1	-15.7	33.9	-15.4	28.7	0.0	-13.5	6.4	-12.7	-10.1	19.1	-7.1	-16.7	2.2	-7.0	67.3	3.5	36.7	16.1	11.5	1.7
-9.6	9.6	1.1	3.9	8.9	11.8	48.1	-21.8	6.5	64.9	-6.3	26.2	-2.0	11.3	12.2	-71.9	26.2	-33.5	44.5	116.5	-65.1	-126.6		
61.0	-163.2		-89.4	46.8	-189.7		-92.6	97.7	-126.3		-119.4		30.4	-134.0		-98.9	81.6	-197.1		-111.1		110.3	1.0
90.9	45.6	-0.9	5.6	24.7	7.5	-1.6	-5.8	3.4	-6.1	0.0	-12.9	-3.4	11.9	-5.7	-32.8	4.3	-17.7	-31.8	22.6	-15.2	-18.1	20.3	-0.3
-11.4	8.8	1.0	37.5	41.7	-15.7	-23.1	-23.9	-2.8	-2.9	-9.4	-4.7	-18.2	4.7	-6.1	-10.0	4.9	-0.8	5.1	-6.1	0.2	-5.6	-22.4	
Avg dipropylamine			5.6	-14.2	34.9	-19.9	26.1	0.4	-17.7	4.9	-16.1	-15.9	14.6	-12.7	-20.3	-1.7	-10.1	62.1	-0.8	32.6	17.8	11.3	
2.1	-14.0	8.1	-1.2	0.9	5.3	4.6	46.7	-24.7	6.0	58.9	-9.5	23.5	-6.3	5.6	9.6	-71.5	27.4	-35.4					

n,n-dimethylbenzylamine 1	1.3	-14.5	19.6	-17.7	12.6	-5.9	-14.4	2.2	-16.8	-16.7	6.6	-24.1	-13.7	0.5	-14.2	28.9	-5.5	-22.1	19.0						
17.4	5.9	-8.7	12.3	6.5	3.8	7.0	7.0	47.4	-21.3	15.1	64.9	-3.3	27.3	-9.3	9.0	6.0	-11.3	91.3	-50.3	45.0	113.3	-73.6	-		
127.4	-92.8	57.8	-139.8		-74.4	19.9	-185.0		-90.0	79.2	-129.1		-113.4	25.5	-127.8		-89.1	76.5	-183.0		-101.7				
102.3	0.3	81.2	34.3	0.9	1.6	10.6	-3.0	1.0	3.5	-3.4	-2.4	10.1	-25.4	-20.5	11.0	-2.6	-30.2	6.4	-21.2	-31.4	23.4	-19.5	-18.1		
18.2	0.8	-9.3	2.5	1.3	4.8	-6.0	-19.3	-16.8	-14.3	-5.0	2.4	-2.7	-0.3	-7.5	5.1	-1.8	-8.7	3.8	-0.6	3.3	3.2	1.5	0.4		
-9.9																									
Avg n,n-dimethylbenzylamine	3.4	-10.4	27.4	-15.5	17.7	-0.3	-15.2	7.5	-17.8	-16.3	10.0	-22.3	-12.2	6.1	-5.5	31.7	-1.3	-12.6	18.2						
15.8	7.6	-10.4	10.0	2.6	1.7	4.4	4.7	46.8	-20.6	12.2	62.5	-5.7	24.8	-13.6	7.7	9.1	-15.7	90.9	-54.2	50.7	112.4	-85.8	-		
129.7	-95.6	58.2	-141.0		-73.7	13.0	-187.7		-91.8	77.7	-132.3		-116.7	21.8	-131.8		-91.9	79.2	-190.1		-106.2				
101.7	0.7	78.7	34.2	-0.6	1.0	9.8	-1.5	0.5	4.0	-3.1	-2.6	8.1	-22.7	-19.9	11.4	-3.6	-28.0	5.7	-20.8	-31.6	23.9	-16.5	-15.2		
17.4	0.0	-8.7	5.6	0.3	7.0	1.5	-17.5	-16.8	-15.8	-3.8	3.0	-3.5	-1.3	-6.0	6.0	-0.6	-7.1	7.0	-0.1	7.8	2.3	0.7	5.3		
-2.4																									
undecylamine 3	6.1	-7.6	21.3	-17.9	26.7	1.7	-14.4	21.6	-17.8	-0.9	18.4	-14.9	1.5	-3.5	10.8	56.9	-3.9	28.8	5.9	-0.2	-13.8				
-11.7	7.0	6.6	-8.8	6.3	-1.9	74.3	-26.3	21.2	51.2	-5.0	33.1	3.0	2.5	6.3	-88.6	3.2	-18.6	-15.0	68.0	-53.1	-125.9	-83.5			
98.4	-171.7		-86.0	82.0	-179.5		-80.9	82.3	-131.5		-90.3	72.5	-131.4		-82.2	100.8	-195.5		-100.2		119.7	1.0	80.5		
42.8	-1.0	14.9	18.2	-6.3	-3.0	15.1	-2.0	-4.1	16.9	-9.2	-1.4	3.4	-6.8	-35.7	6.3	-24.9	-37.6	40.7	-39.9	-33.7	48.6	0.1	-6.8		
10.8	-0.8	21.7	24.9	-17.2	-29.4	-20.1	-12.3	-24.9	-9.3	-1.4	-3.2	-2.4	-3.2	-6.9	-4.8	0.7	-1.5	-3.1	0.0	8.0	-1.8				
undecylamine 2	0.9	-13.0	15.2	-26.3	22.5	-4.3	-22.5	17.0	-24.8	-6.8	15.5	-22.4	-8.7	-3.9	2.0	57.2	-6.6	31.8	1.3	-3.1	-10.5				
-18.9	-2.4	-1.1	-14.8	-2.1	-7.0	68.4	-27.1	23.0	50.9	-9.2	23.6	-1.5	0.9	3.8	-94.9	2.3	-15.9	-23.5	59.8	-50.6	-126.9	-82.9			
92.8	-169.4		-82.5	80.4	-180.4		-80.9	76.1	-129.2		-93.6	68.5	-115.6		-69.9	95.4	-197.0		-95.4	112.7	-0.8	73.9	35.8		
-0.6	13.5	18.1	-4.9	-3.5	8.7	-2.9	-5.4	14.7	-8.8	-1.8	5.0	-8.0	-34.6	11.6	-20.0	-33.1	46.6	-32.1	-29.9	50.2	-0.3	-3.9	11.8		
-0.8	21.1	21.6	-10.2	-23.3	-16.2	-3.5	-16.0	-7.1	3.5	4.5	2.8	2.1	-1.0	1.0	-0.4	4.2	0.3	0.2	12.3	3.1					
undecylamine 1	0.3	-13.1	16.9	-35.1	22.5	-1.2	-21.5	15.9	-23.8	-7.4	10.7	-26.0	-16.0	-6.0	-0.6	56.0	-9.6	25.6	1.3	-2.6	-14.5				
-17.8	0.3	-0.9	-18.3	-5.4	-10.2	66.6	-32.5	18.7	44.2	-11.6	22.9	-5.6	-2.9	-0.2	-85.4	6.5	-16.1	-23.6	59.8	-54.6	-119.4	-80.4			
86.5	-165.2		-83.6	75.0	-169.9		-80.6	76.3	-124.3		-92.7	66.9	-118.7		-72.5	93.9	-185.7		-92.6	108.8	-0.1	70.3	34.1		
-3.3	14.9	14.4	-5.7	-1.6	4.3	-2.8	-3.5	11.7	-7.7	0.3	5.3	-10.5	-34.6	10.1	-22.6	-26.1	40.8	-30.8	-25.4	49.1	0.2	-4.0	14.1		
Avg undecylamine	2.4	-11.2	17.8	-26.4	23.9	-1.3	-19.5	18.2	-22.1	-5.1	14.9	-21.1	-7.7	-4.5	4.1	56.7	-6.7	28.7	2.8	-2.0					
-12.9	-16.2	1.6	1.5	-14.0	-0.4	-6.4	69.8	-28.6	20.9	48.8	-8.6	26.6	-1.4	0.2	3.3	-89.6	4.0	-16.8	-20.7	62.5	-52.8	-124.0			
-82.3	92.6	-168.8		-84.1	79.1	-176.6		-80.8	78.2	-128.3		-92.2	69.3	-121.9		-74.9	96.7	-192.7		-96.1	113.7	0.0	74.9		
37.6	-1.6	14.4	16.9	-5.7	-2.7	9.4	-2.5	-4.4	14.4	-8.6	-1.0	4.6	-8.4	-34.9	9.3	-22.5	-32.3	42.7	-34.3	-29.7	49.3	0.0	-4.9		
12.3	0.2	21.5	23.1	-11.6	-23.3	-15.2	-8.7	-20.1	-9.4	0.6	-0.3	0.4	-0.5	-3.2	-0.5	0.1	3.0	-1.1	0.3	11.3	2.0				
n-octylamine 2	-1.1	-30.4	15.5	-35.3	26.6	-6.4	-44.1	6.5	-30.3	-18.8	11.8	-34.2	44.7	-5.0	27.9	69.4	-8.4	28.2	18.0	6.8	-14.3				
-27.4	0.0	-4.3	-14.6	2.6	-9.6	37.4	-29.0	-1.3	59.5	-9.8	20.8	-5.2	-4.9	-3.2	-97.7	6.5	-12.7	2.2	91.7	-46.6	-110.2	-78.6			
60.6	-160.7		-82.5	62.7	-181.2		-86.6	109.4	-118.0		-105.6	49.2	-112.2		-77.1	82.0	-192.1		-99.2	118.3	0.1	79.5			
38.8	-2.3	-2.6	32.6	7.1	10.1	-7.4	13.4	9.1	5.1	-21.8	-13.4	19.6	-13.4	-24.9	21.9	-25.3	-24.6	44.5	-25.2	-16.9	53.3	-0.8	-1.9		
23.7	0.8	42.3	55.1	-12.3	-7.4	-5.7	25.7	28.8	11.1	-1.4	-13.7	9.7	8.9	-0.5	18.3	2.2	13.6	1.2	0.7	-1.2	-17.4				
n-octylamine 1	-5.8	-32.5	9.4	-36.6	23.2	-6.9	-41.3	5.0	-31.7	-21.8	17.0	-28.8	50.2	-5.3	24.8	74.2	-3.0	31.6	15.3	6.2	-10.4				
-21.9	5.4	-3.3	-10.4	2.1	-7.1	39.0	-32.2	1.7	59.8	-4.2	24.4	-3.0	-1.2	-2.6	-98.4	12.3	-3.9	5.5	97.6	-40.3	-112.8	-74.9			
69.2	-169.3		-83.6	67.4	-187.5		-89.7	110.3	-124.0		-108.7	41.3	-126.6		-78.9	93.2	-194.7		-96.3	123.4	0.8	87.8			
46.5	-6.8	-0.4	30.3	5.9	9.0	-9.4	14.8	5.8	1.6	-22.4	-15.2	21.2	-10.8	-33.6	16.2	-27.7	-31.1	40.1	-25.8	-19.7	48.6	-0.1	-4.4		
19.1	-2.3	41.5	54.4	-24.0	-18.4	-15.8	10.9	11.4	0.3	-9.6	-21.9	1.4	0.7	-5.1	11.7	1.3	9.0	-7.3	0.2	-6.9	-22.8				
n-octylamine 3	1.4	-31.2	21.1	-34.8	29.3	-4.2	-45.7	12.3	-25.9	-15.9	14.4	-28.7	53.9	-3.9	30.9	75.8	-3.3	28.7	10.8	2.9	-14.4				
-26.7	0.4	-3.8	-9.0	6.1	-6.9	41.7	-21.3	7.1	64.4	-3.5	28.8	0.5	0.5	-5.4	-106.5	4.4	-13.0	-23.6	60.9	-68.1	-115.2				
-78.1	68.5	-163.6		-79.6	73.2	-181.5		-84.4	117.7	-117.1		-104.3	53.7	-131.4		-85.0	95.0	-193.4		-99.1	122.8	0.3			
87.5	47.1	-1.3	2.4	36.8	8.8	9.8	-0.6	11.9	7.1	5.4	-23.1	-12.3	19.4	-13.3	-33.6	20.8	-30.7	-32.3	41.5	-28.5	-18.9	51.6	-0.1	-4.4	
-6.9	17.9	-1.9	40.7	48.4	-14.3	-11.8	9.1	9.1	11.3	12.2	2.9	-4.1	-17.4	4.5	2.1	-10.7	7.8	0.1	4.8	-8.9	-0.8	-12.4	-25.8		
Avg n-octylamine	-1.8	-31.4	15.4	-35.6	26.4	-5.8	-43.7	7.9	-29.3	-18.8	14.4	-30.6	49.6	-4.7	27.9	73.1	-4.9	29.5	14.7	5.3	-13.1				
-25.3	2.0	-3.8	-11.4	3.6	-7.9	39.4	-27.5	2.5	61.2	-5.8	24.7	-2.6	-1.8	-3.7	-100.8	7.7	-9.9	-5.3	83.4	-51.7	-112.7				
-77.2	66.1	-164.5		-81.9	67.8	-183.4		-86.9	112.5	-119.7		-106.2	48.1	-123.4		-80.3	90.0	-193.4		-98.2	121.5	0.4			
84.9	44.1	-3.5	-0.2	33.2	7.3	9.6	-5.8	13.4	7.3	4.0	-22.4	-13.6	20.1	-12.5	-30.7	19.6	-27.9	-29.3	42.0	-26.5	-18.5	51.2	-0.4		
-4.4	20.2	-1.2	41.5	52.6	-16.9	-12.6	-10.2	16.0	17.4	4.8	-5.1	-17.7	5.2	3.9	-5.4	12.6	1.2	9.2	-5.0	0.0	-6.8	-22.0			
diisobutylamine avg	2.4	-3.1	19.1	5.8	33.7	14.4	-9.7	29.2	-6.6	-3.2	28.2	-2.4	5.9	24.2	23.1	39.3	10.6	40.6	24.5	19.5					
12.5	-4.1	11.3	18.4	2.1	8.1	11.6	50.4	-14.4	42.7	44.6	11.4	52.5	0.5	15.7	24.4	-56.8	40.1	-21.8	32.5	100.1	-49.5	-118.0			
-83.4	95.7	-180.4		-86.3	71.4	-191.8		-96.2	55.5	-137.0		-94.4	77.9	-71.7	-57.7	88.5	-202.3		-97.4	117.1	-4.7	73.8	31.0		
-10.9	10.1	8.4	-9.6	-8.5	6.5	-6.3	-10.8	6.9	-6.3	-2.2	-1.3	-17.0	-36.7	3.5	-29.4</										

nonylamine 2	1.8	-17.8	17.1	-13.4	30.6	-10.3	-21.3	24.5	-21.3	-3.8	22.9	-25.1	24.4	-12.8	14.4	53.6	-4.8	27.3	13.0	2.9	-14.4				
	-17.2	4.5	7.0	-15.2	1.1	-7.3	51.1	-34.8	16.2	30.5	-1.8	30.5	-3.3	-5.9	-2.5	-100.3	12.3	18.0	-9.6	73.9	-33.1	-113.2			
	-70.4	100.6	-166.3		-84.9	90.1	-176.7		-76.9	85.5	-125.8		-89.6	74.3	-97.5	-59.4	96.8	-201.0		-89.1	120.3	-4.2	76.5	39.0	
	-7.0	14.3	21.8	-12.1	-8.9	15.2	-4.1	-7.8	18.9	-8.7	1.7	8.4	-17.5	-37.2	4.0	-29.5	-36.7	36.6	-39.0	-36.5	53.9	-3.8	-11.7	12.0	
	-6.3	27.5	26.8	-18.2	-33.9	-20.5	-18.9	-33.4	-16.2	-5.2	-6.5	-7.4	-6.7	-9.7	-8.3	1.5	3.5	0.6	2.0	9.9	3.1				
t-octylamine avg	-0.3	-7.2	19.2	-11.9	32.2	10.6	-20.6	20.2	-4.7	-7.8	22.0	-7.8	-1.2	14.4	14.2	38.9	7.8	34.3	24.0	19.4	3.7				
	-11.9	8.8	14.8	-4.9	1.0	4.7	26.0	-19.3	27.9	22.1	13.9	35.0	1.5	10.9	22.0	-73.9	16.5	18.3	13.8	83.3	-15.9	-112.4	-80.5		
	84.6	-129.8		-95.6	71.3	-183.2		-77.9	78.9	-119.4		-88.1	80.2	-103.7	-75.5	94.7	-191.8		-92.2	119.7	-3.1	65.7	43.4		
	-5.9	17.3	34.1	-5.3	-4.6	10.8	-2.7	-7.6	13.0	-2.1	2.6	7.0	-5.5	-21.4	1.9	-16.0	-19.0	23.0	-14.2	-13.7	30.5	0.6	-8.8	7.4	
	-10.9	22.4	29.4	-10.8	-20.6	-14.0	-5.0	-14.9	-12.8	-3.6	-11.9	-1.3	-7.1	-3.5	1.7	0.5	7.9	1.1	0.6	7.8	12.8				
t-octylamine 1	-1.2	-7.8	17.7	-13.5	31.5	10.2	-20.5	17.4	-3.9	-7.0	19.8	-8.1	-1.0	13.4	13.3	42.4	10.1	38.0	22.4	18.8	2.8				
	-12.0	8.5	10.8	-5.0	-0.4	4.6	16.2	-26.3	15.3	24.4	11.4	36.0	-1.3	10.7	20.3	-72.0	16.7	15.3	8.7	79.1	-11.8	-111.8	-79.7		
	78.2	-132.5		-100.7	65.4	-184.2		-78.5	80.1	-120.2		-90.0	71.2	-100.9	-75.3	93.6	-192.4		-93.0	120.0	-1.5	69.1			
	43.2	-6.0	18.4	32.4	-4.3	-4.4	8.7	-0.5	-6.4	10.9	0.0	4.7	8.8	-5.8	-21.2	2.8	-14.9	-18.1	20.5	-14.7	-15.7	30.3	2.3	-8.9	
t-octylamine 3	0.6	-6.6	20.7	-10.3	32.9	11.0	-20.6	22.9	-5.4	-8.6	24.1	-7.5	-1.5	15.3	15.1	35.3	5.5	30.5	25.5	20.0	4.5				
	-11.8	9.1	18.9	-4.9	2.4	4.8	35.7	-12.4	40.4	19.7	16.4	34.0	4.4	11.0	23.7	-75.7	16.2	21.3	18.9	87.5	-19.9	-113.0	-81.4		
	90.9	-127.0		-90.5	77.1	-182.2		-77.2	77.6	-118.6		-86.3	89.2	-106.4	-75.8	95.9	-191.2		-91.4	119.4	-4.6	62.3	43.6		
	-5.8	16.3	35.7	-6.4	-4.8	13.0	-4.9	-8.8	15.1	-4.1	0.6	5.1	-5.2	-21.6	1.0	-17.1	-20.0	25.6	-13.6	-11.6	30.7	-1.2	-8.7	8.0	
	-12.3	21.3	26.5	-13.9	-23.4	-16.5	-10.0	-18.5	-13.9	-6.3	-14.4	-2.6	-9.2	-11.3	-6.4	-0.4	7.9	-0.6	1.3	7.3	10.9				
heptylamine avg	1.4	-16.7	18.3	-17.5	27.6	-10.0	-24.8	18.2	-23.7	-10.2	18.1	-27.3	26.7	-13.4	17.0	48.9	-7.9	25.1	14.8	6.7	-10.9				
	-15.6	5.2	7.1	-14.6	0.6	-5.9	52.0	-21.5	33.9	37.4	-4.1	33.1	-2.9	-4.5	-0.2	-100.6	15.4	14.3	-19.2	66.4	-28.6	-111.3			
	-70.0	89.7	-161.3		-80.0	89.0	-173.3		-73.8	84.2	-125.9		-86.0	77.8	-98.1	-61.2	89.0	-194.5		-86.5	122.8	-5.1	84.1	40.6	
	-7.9	13.2	24.6	-6.2	-1.7	13.0	3.3	-0.1	15.2	-5.8	1.5	11.3	-15.3	-30.3	11.9	-29.1	-35.3	41.3	-34.4	-29.3	66.3	-4.3	-4.8	16.3	
heptylamine 1	1.4	-16.3	17.4	-17.7	29.3	-9.0	-24.2	20.4	-24.2	-7.7	22.0	-24.5	29.9	-9.8	20.7	51.9	-5.2	28.2	18.2	9.1	-8.6				
	-15.7	7.2	8.3	-13.7	2.9	-5.0	55.8	-22.1	34.4	46.5	-2.6	37.8	0.6	0.3	2.5	-100.8	20.7	15.2	-17.1	69.5	-27.1	-111.2			
	-68.0	89.2	-161.5		-76.6	90.0	-174.1		-70.6	89.8	-128.3		-86.0	75.8	-100.7		-61.1	84.7	-190.6		-85.9	123.4	-4.1	84.5	
	40.1	-10.5	14.1	22.6	-5.6	-2.9	11.2	4.5	0.8	11.1	-5.0	0.3	10.2	-16.1	-27.7	12.8	-27.2	-34.2	35.2	-33.1	-27.3	63.1	-5.4	-4.8	
	16.0	-7.1	28.2	33.0	-15.4	-27.0	-18.6	-16.4	-27.1	-16.7	-3.6	-7.2	-5.9	-6.4	-9.1	-5.6	13.9	0.5	-3.3	-0.3	12.5	-0.2			
heptylamine 2	1.5	-16.8	18.7	-15.8	27.8	-10.0	-22.9	18.4	-21.5	-8.4	17.3	-25.3	28.0	-15.3	16.6	51.3	-8.4	22.5	12.1	4.8	-12.4				
	-15.7	3.8	4.9	-15.9	-0.2	-7.2	53.0	-21.5	34.2	37.5	-7.6	33.1	-4.6	-8.6	-2.8	-103.3	12.5	9.7	-17.2	66.0	-31.6	-116.3			
	-75.3	89.7	-159.7		-84.1	83.0	-174.3		-77.6	81.1	-127.2		-90.7	73.5	-97.6	-62.9	88.9	-197.9		-90.6	119.8	-4.2	85.6	40.7	
	-3.9	13.8	22.5	-9.7	-3.6	11.9	1.5	-1.9	14.3	-5.2	3.2	11.2	-12.9	-33.1	7.9	-29.4	-35.4	44.9	-34.5	-31.2	61.9	-3.4	-3.8	11.8	
heptylamine 3	1.5	-16.9	18.8	-18.9	25.6	-10.9	-27.2	15.7	-25.3	-14.5	15.0	-32.2	22.0	-15.1	13.6	43.5	-10.2	24.4	14.1	6.2	-11.7				
	-15.2	4.8	8.0	-14.2	-1.0	-5.5	47.3	-20.9	33.1	28.3	-2.2	28.5	-4.8	-5.3	-0.3	-97.6	12.9	17.9	-23.2	63.6	-27.3	-106.5	-66.7		
	90.1	-162.8		-79.4	94.1	-171.4		-73.3	81.7	-122.3		-81.2	84.2	-95.8	-59.7	93.2	-195.0		-83.0	125.1	-7.0	82.2	41.0	-9.4	
	11.8	28.6	-3.3	1.3	15.8	3.8	0.7	20.3	-7.2	1.1	12.5	-17.0	-30.1	15.1	-30.6	-36.3	43.8	-35.7	-29.5	73.9	-3.9	-5.8	21.1	-8.9	
aniline 1	2.6	-11.6	15.1	-19.5	21.7	-10.6	-15.6	16.7	-15.0	-7.4	16.2	-43.8	-2.9	-7.8	1.7	46.0	9.1	26.0	0.1	-4.3	-13.1	-12.2			
	-0.9	0.8	-8.9	-0.2	-23.6	54.5	-28.9	31.5	47.0	-13.7	25.0	-2.2	-3.5	5.0	0.6	119.0	-63.7	49.9	115.9	-69.4	-122.1		-80.6	51.1	
	1.8	10.8	-13.7	-27.0	-42.7	-5.5	-86.4	-39.4	-12.8	-113.9		-76.2	55.2	-168.0		-84.3	23.4	-2.3	-1.4	8.4	-3.3	3.9	-3.8	-9.4	
	0.2	-2.6	-8.8	-0.3	-0.4	-5.1	-2.5	-7.3	-6.7	-6.9	-0.5	-10.7	-5.2	-2.0	-13.6	-4.9	-3.3	-0.1	8.0	-1.5	-6.5	-5.5	-0.7	-3.2	
aniline 2	6.4	-7.9	20.4	-14.0	25.8	-2.7	-11.4	21.6	-4.7	1.5	19.0	-32.7	-2.3	-2.3	2.4	47.1	-6.3	27.6	1.4	-0.9	-7.2	-8.2			
	4.4	9.1	-4.1	3.7	-15.7	61.7	-25.7	36.7	47.5	-7.7	29.4	-0.9	-2.0	4.6	-0.2	123.5	-69.5	52.2	122.6	-64.5	-117.5		-74.8	56.9	
	2.1	16.7	-11.3	-27.1	-42.4	-3.6	-87.1	-37.6	-8.8	-116.9		-74.6	59.8	-165.4		-82.2	32.3	0.7	3.9	14.1	0.0	11.5	3.2	-7.3	
	3.8	2.9	-7.3	3.4	4.5	-2.7	0.7	-1.2	0.8	-5.3	4.1	-4.3	2.1	5.2	-13.4	-5.4	2.7	0.0	-0.2	0.5	-0.7	-1.8	0.0	0.8	
aniline 3	0.8	-10.2	12.9	-17.8	22.2	-6.0	-15.6	17.3	-14.3	-4.6	13.6	-42.4	-1.6	-9.7	-4.2	45.9	-9.0	23.6	0.6	-1.6	-11.8	-10.8			
	4.0	2.4	-5.1	0.7	-22.5	53.1	-29.1	23.6	43.6	-14.0	21.3	-2.4	-5.4	-3.9	2.2	125.2	-68.6	49.4	117.5	-64.3	-111.6		-72.6	51.9	
	-0.6	15.7	-14.0	-24.1	-43.0	-14.1	-82.5	-40.5	-8.9	-111.3		-71.9	56.1	-158.3		-76.6	26.2	-0.9	5.9	9.1	-0.4	11.6	-3.4	-5.4	
	2.8	-2.7	7.2	1.9	0.3	-3.2	2.8	-0.6	-1.8	2.5	-4.9	2.9	2.1	-8.1	-0.3	-2.8	-0.8	-2.8	-2.2	-1.3	-2.4	0.7	0.9		
	4.3	0.6	-12.1	6.1	1.8	1.0	-2.1	0.7	-19.7	-14.7	16.7	-3.9	1.2	0.2	0.1	-25.2	-43.3								
aniline avg	3.3	-9.9	16.1	-17.1	23.3	-6.4	-14.2	18.6	-11.3	-3.5	16.3	-39.6	-2.3	-6.6	0.0	46.3	-8.1	25.7	0.7	-2.2	-10.7	-10.4			
	2.5	4.1	-6.0	1.4	-20.6	56.5	-27.9	30.6	46.0	-11.8	25.2	-1.8	-3.6	1.9	0.8	122.5	-67.3	50.5	118.7	-66.1	-117.0		-76.0	53.3	
	1.1	14.4	-13.0	-26.1	-42.7	-7.7	-85.3	-39.2	-10.2	-114.0		-74.2	57.0	-163.9		-81.0	27.3	-0.8	2.8	10.5	-1.2	9.0	-1.3	-7.4	
	2.3	-0.8	-7.8	1.6	1.5	-3.7	0.3	-3.0	-2.2	-4.7	2.1	-6.6	0												

-87.0	81.9	-168.6	-88.3	79.5	-195.3	-101.5	73.8	-138.7	-107.6	64.3	-119.0	-77.0	80.3	-198.5	-102.0										
117.9	91.1	83.8	40.4	-1.6	20.4	16.7	-8.0	-5.9	11.9	-5.0	-10.4	14.5	-5.5	1.3	4.4	-13.5	-43.5	7.2	-26.2	-38.4	40.3	-42.2	-43.4		
49.4	-0.3	-7.6	6.7	-1.3	18.0	19.1	-7.8	-18.4	-12.1	-7.8	-17.9	-11.0	-1.7	-4.5	-5.5	-4.1	-8.0	-6.2	6.0	3.8	-1.1	0.4	14.6		
5.8																									
disecbutylamine 2		5.2	-3.3	26.2	-7.6	30.9	14.7	-12.5	20.0	-5.6	1.5	18.1	-2.7	-3.0	13.4	11.2	36.1	7.1	19.6	17.2	15.6	6.5			
	-4.7	9.4	13.4	0.4	6.2	10.2	64.0	-21.8	58.1	54.3	-4.1	49.9	3.5	-2.7	12.7	-68.1	39.2	-41.5	36.4	103.2	-55.3	-127.6	-78.6		
	81.4	-164.7	-78.1	78.3	-186.8	-93.9	65.2	-130.1	-92.8	67.2	-117.9	-70.7	78.8	-198.1	-93.0	124.2	0.4	77.1	36.6						
	-1.6	20.4	14.1	9.0	-2.5	12.5	-6.0	-8.3	18.8	-6.2	-1.3	4.0	-12.7	-40.3	6.7	-25.2	-39.4	36.5	-38.9	-38.7	36.2	-0.1	-5.5	8.4	
	-2.1	9.8	10.6	-9.3	-17.3	-6.9	-9.2	-13.9	-4.3	-3.3	-5.0	-5.4	-9.9	-8.6	-6.6	7.7	3.1	-1.8	0.5	14.4	7.2				
disecbutylamine 1		3.2	-1.0	20.0	-7.7	29.6	17.3	-16.1	15.7	-2.7	-3.5	15.8	3.1	-1.4	15.5	14.8	36.2	9.5	18.8	21.8	19.7	12.8			
	-7.8	14.4	14.6	0.0	7.2	15.8	61.8	-24.7	60.1	55.1	-2.2	60.7	2.0	0.1	12.3	-69.7	41.5	-36.4	35.4	109.2	-52.7	-123.2	-77.7		
	71.7	-164.1	-79.4	86.2	-185.6	-94.2	70.7	-128.2	-97.1	64.3	-120.0	-69.8	73.2	-193.2	-88.8	129.6	2.2	81.3	38.4						
	-2.8	23.3	18.4	-6.0	-2.2	15.7	-1.7	-6.2	17.7	-1.5	4.6	4.3	-9.5	-39.5	9.6	-22.9	-33.0	48.2	-37.8	-37.3	45.7	-0.3	-3.4	13.7	
	-1.2	12.4	12.6	-6.2	-12.9	-1.3	-6.8	-10.6	-0.3	1.9	2.5	3.5	-1.6	-6.1	3.4	10.9	7.4	1.0	0.7	21.4	16.8				
disecbutylamine 3		7.2	5.1	21.8	-1.0	39.0	25.6	-14.3	22.3	-9.0	1.6	18.8	-2.7	8.2	22.8	19.1	46.8	17.6	30.5	23.0	21.9	12.0			
	-5.5	17.6	19.4	4.4	12.1	17.9	66.6	-22.6	55.2	68.4	6.4	67.8	9.8	19.2	29.4	-77.0	36.7	-37.5	30.0	108.6	-58.9	-126.4	-80.6		
	73.3	-164.1	-80.0	85.6	-183.8	-96.3	72.3	-124.8	-95.4	69.7	-120.7	-72.0	74.9	-195.9	-92.7	129.4	1.0	79.2	36.0						
	-0.6	21.5	17.9	-5.0	-1.2	13.5	-1.8	-7.2	11.6	-4.8	2.1	8.3	-12.4	-41.8	6.1	-25.6	-39.8	46.1	-39.8	-42.0	45.7	0.1	-4.1	9.8	
	-0.1	11.1	9.1	-9.8	-14.4	-3.3	-7.6	-11.0	-0.8	0.7	-0.2	-1.5	-6.3	-9.4	-4.0	4.5	4.5	1.1	0.2	20.4	9.1				
disecbutylamine avg		5.2	0.3	22.7	-5.4	33.2	19.2	-14.3	19.3	-5.8	-0.1	17.6	-0.8	1.3	17.2	15.0	39.7	11.4	23.0	20.7	19.1				
	10.4	-6.0	13.8	15.8	1.6	8.5	14.6	-23.0	57.8	59.3	0.0	59.5	5.1	5.5	18.1	-71.6	39.1	-38.5	33.9	107.0	-55.6	-125.7			
	-79.0	75.5	-164.3	-79.2	83.4	-185.4	-94.8	69.4	-127.7	-95.1	67.1	-119.5	-70.9	75.6	-195.7	-91.5	127.7	1.2	79.2						
	37.0	-1.7	21.7	16.8	-6.7	-2.0	13.9	-3.2	-7.2	16.0	-4.1	1.8	5.5	-11.5	-40.5	7.5	-24.6	-37.4	43.6	-38.8	-39.3	42.5	-0.1	-4.3	
	10.6	-1.2	11.1	10.8	-8.5	-14.8	-3.8	-7.9	-11.8	-1.8	-0.2	-0.9	-1.1	-5.9	-8.0	-2.4	7.7	5.0	0.1	0.5	18.7	11.1			
triethylamine 3		1.8	5.3	5.5	-18.1	14.5	14.2	-6.7	14.0	-9.6	0.2	10.8	-9.9	-16.1	-2.3	-8.0	16.4	-7.7	-12.7	3.7	3.8	-5.0			
	-5.0	8.0	1.4	-0.3	4.7	0.2	66.8	-40.2	32.1	48.8	-14.6	37.7	0.0	0.2	2.9	-24.8	96.4	-53.2	49.9	120.0	-58.7	-130.2	-90.2		
	86.9	-141.3	-67.0	33.9	-183.4	-99.4	64.0	-129.6	-97.4	53.0	-115.4	-82.1	92.8	-192.4	-104.8	117.5	-0.5	83.5							
	34.8	-1.6	23.3	9.0	-3.3	-1.4	9.4	-0.8	-3.6	8.7	-1.6	3.1	9.9	-6.5	-20.2	7.2	-16.3	-20.5	22.8	-19.4	-17.1	18.1	-0.5	-3.5	
	5.2	-0.2	5.8	6.5	-4.3	-11.6	-7.3	-8.1	-12.7	-10.0	-0.7	-1.3	-3.4	-3.5	-5.4	-6.5	-1.5	-1.2	-1.8	0.6	9.3	-1.6			
triethylamine 2		1.6	1.9	3.4	-16.2	8.9	9.9	-6.9	10.6	-7.7	-2.5	7.6	-11.2	-17.6	-1.4	-7.7	16.6	-8.5	-15.8	4.6	2.8	-7.0			
	-6.4	5.0	-1.3	-0.6	1.1	1.2	62.3	-39.1	31.4	50.0	-15.4	34.3	-0.1	0.5	0.8	-4.5	115.4	-65.6	47.6	118.4	-58.9	-130.0	-91.5		
	89.6	-109.0	-40.5	11.1	-185.5	-91.3	44.8	-132.4	-94.9	40.4	-120.7	-88.4	97.6	-196.4	-107.6	110.7	-0.4	70.6							
	26.5	-1.9	22.1	6.6	-4.0	-0.5	7.3	-3.1	-2.8	11.0	-2.0	-0.2	4.0	-4.8	-13.4	3.1	-11.8	-15.5	16.9	-16.5	-13.0	11.9	-2.1	-2.9	
	3.6	-1.1	4.0	3.2	-5.7	-15.0	-9.1	-8.6	-10.6	-8.3	1.4	-0.6	-3.2	-0.2	-3.8	-4.2	3.1	-0.3	0.5	-0.2	11.6	-0.8			
triethylamine 1		12.5	13.7	11.8	-5.0	18.1	18.3	5.3	18.2	0.6	7.5	13.6	-1.5	-11.1	5.0	-2.6	20.2	-4.2	-11.4	10.7	9.5	-7.2			
	7.6	16.1	9.9	9.8	12.4	8.3	68.9	-33.9	27.8	53.4	-8.7	40.5	6.0	7.4	6.3	-3.7	113.1	-60.4	62.0	122.9	-50.2	-122.1	-80.9		
	95.0	-123.2	-50.5	27.6	-180.4	-89.6	54.4	-124.9	-88.8	55.2	-116.8	-81.7	94.5	-192.7	-99.9	116.7	12.8	86.4	35.7						
	9.5	30.2	13.7	1.2	2.6	19.6	0.9	-0.5	20.9	7.3	7.2	11.3	5.6	-13.2	5.7	-5.7	-14.4	29.6	-14.8	-13.3	20.9	9.5	4.0	10.2	
	6.2	9.5	6.6	2.7	-1.6	-4.6	1.5	-5.3	-1.8	10.9	7.6	2.5	7.1	2.4	1.2	15.5	4.4	7.2	6.0	14.5	5.1				
triethylamine average		5.3	7.0	6.9	-13.1	13.8	14.2	-2.8	14.3	-5.6	1.7	10.7	-7.5	-14.9	0.4	-6.1	17.7	-6.8	-13.3	6.3	5.4				
	-6.4	-1.3	9.7	3.3	3.0	6.0	3.2	66.0	-37.7	30.5	50.7	-12.9	37.5	2.0	2.7	3.3	-11.0	108.3	-59.7	53.1	120.4	-55.9	-127.4		
	-87.6	90.5	-124.5	-52.7	24.2	-183.1	-93.4	54.4	-128.9	-93.7	49.5	-117.7	-84.1	95.0	-193.8	-104.1	115.0	3.9							
	80.2	32.3	2.0	25.2	9.8	-2.0	0.2	12.1	-1.0	-2.3	13.6	1.2	3.4	8.4	-1.9	-15.6	5.3	-11.3	-16.8	23.1	-16.9	-14.5	16.9	2.3	
	-0.8	6.3	1.6	6.4	5.4	-2.4	-9.4	-7.0	-5.1	-9.5	-6.7	3.9	1.9	-1.4	1.1	-2.2	-3.2	5.7	1.0	2.0	2.1	11.8	0.9		
1,5-dimethylhexylamine 1		2.1	-4.9	24.7	-6.0	38.1	14.7	-12.4	28.8	-3.1	-1.2	33.2	-4.8	16.7	11.4	27.7	55.2	17.4	56.6	25.3					
	20.1	1.1	-7.1	12.1	22.4	-3.1	9.6	6.4	41.9	-13.1	36.6	24.9	10.5	38.7	2.6	14.4	23.1	-78.7	8.5	35.9	14.9	88.1	-6.4	-	
	111.2	-76.8	90.0	-153.6	-81.5	105.6	-186.2	-80.3	88.8	-121.7	-88.3	92.7	-116.8	-80.1	103.9	-191.5	-83.1	133.4	-4.2						
	73.5	44.7	-6.0	24.8	32.9	-3.8	-3.1	16.7	0.3	-4.9	18.8	-5.0	-2.3	7.8	-13.9	-26.6	10.0	-22.0	-23.5	35.6	-24.8	-20.1	54.1	-1.3	
	-8.4	17.0	-5.9	31.5	35.5	-18.1	-27.0	-17.3	-13.7	-21.8	-15.7	-6.9	-16.6	1.4	-8.2	-8.7	4.5	-0.3	5.1	1.6	0.8	7.8	6.6		
1,5-dimethylhexylamine 2		-4.1	-11.0	16.2	-12.8	32.9	4.3	-20.6	17.4	-15.7	-9.4	23.6	-17.2	7.1	1.6	19.0	44.4	8.2	46.0	21.5					
	17.2	0.3	-13.2	6.1	14.2	-7.8	1.9	1.7	28.8	-10.1	22.6	3.5	-7.4	8.4	0.2	8.9	18.5	-81.2	-53.4	67.0	-12.3	50.5	15.9	-	
	112.2	-77.0	95.4	-161.0	-86.3	107.3	-183.3	-76.8	91.4	-114.6	-85.2	102.1	-116.4	-79.9	111.3	-188.3	-83.3	141.8	1.0						
	79.9	50.7	1.4	31.0	36.5	-1.5	3.2	23.6	2.2	-1.2	20.4	-1.9	4.6	14.2	-5.3	-25.6	12.3	-15.8	-19.3	42.8	-19.4	-15.4	57.3	0.6	
	-2.3	18.1	-3.6	32.0	31.7	-10.5	-20.1	-13.1	-7.2	-15.4	-11.6	-3.3	-13.9	-0.5	-9.5	-9.1	-0.9	0.1	4.6	0.1	0.4	1.2	3.2		
1,5-dimethylhexylamine 3		1.2	-5.9	20.8	-7.4	40.0	11.5	-13.7	27.9	-7.9	-2.5														

-1.7	2.6	-1.5	-2.4	3.2	-0.3	-0.3	-0.4	-0.8	-7.7	0.8	-5.0	-8.0	4.0	-7.8	-8.8	4.8	0.6	-0.9	0.1	0.6	-0.1	1.8	-1.7			
-1.0	-1.8	-0.6	-1.3	0.0	1.5	-2.6	-3.4	1.4	-0.6	1.0	3.1	-0.7	-3.6	-0.2	9.4	-1.4										
dibenzylamine.avg			0.4	0.8	2.4	-3.6	0.9	0.3	-1.8	2.2	-1.6	0.8	0.4	-0.8	-0.8	0.4	-0.5	2.6	-1.2	-1.4	0.6	0.3				
-1.3	-4.2	1.6	-2.9	-0.2	0.7	-1.1	27.8	-24.0	12.0	48.1	-13.8	31.2	0.7	0.9	0.5	2.8	128.4	-68.1	57.0	114.0	-65.1	-100.6				
-64.2	41.8	3.0	12.5	-7.9	-1.8	-1.3	1.1	-66.5	-20.1	-14.3	-88.8	-56.3	40.9	-127.5	-41.4	16.6	2.1	15.9	-1.2	0.2	7.4	2.7				
-3.7	-2.0	5.6	-2.2	-1.6	5.0	-0.7	-0.9	0.3	-1.6	-7.7	0.1	-6.0	-8.1	5.9	-7.8	-7.9	5.6	-0.1	0.0	1.4	-0.2	1.3	2.7			
-1.7	-1.1	-0.5	-0.4	-0.7	1.1	0.3	-1.8	-2.2	0.3	-0.1	0.6	8.5	-1.1	-1.4	0.3	10.6	-1.4									
dicyclohexylamine 1			-0.1	-12.1	9.8	-23.8	15.8	5.5	-17.2	19.0	-7.9	-2.1	11.7	-9.8	-13.9	-5.7	-8.5	26.0	-8.7	-6.8	1.6	-2.2				
-13.0	-15.7	1.9	-0.2	-6.2	-1.0	-3.0	57.1	-35.9	20.0	38.0	-9.3	32.4	-2.4	0.8	3.3	-91.2	25.1	-26.1	21.6	96.7	-56.4	-139.1				
-81.2	91.3	-180.3	-89.0	81.6	-194.6	-96.7	59.2	-143.1	-94.6	81.9	-125.4	-69.1	88.5	-201.2	-95.3	121.5	-2.2	44.9								
20.9	-5.7	13.5	10.3	-12.6	-7.9	12.5	-5.9	-8.8	16.1	-1.0	-1.5	3.1	-12.9	-34.9	4.5	-27.9	-39.6	34.3	-35.2	-35.1	34.5	-0.4	-5.4			
5.8	-0.7	9.4	7.6	-21.2	-26.2	-11.2	-21.3	-25.1	-12.6	-3.3	-4.9	-5.7	-3.4	-7.4	-8.2	0.2	4.4	2.5	1.1	9.1	1.8					
dicyclohexylamine 2			-0.1	-12.6	10.7	-24.6	15.2	1.3	-21.0	13.9	-16.3	-5.8	8.2	-14.7	-19.6	-10.4	-14.0	22.2	-12.4	-15.5	3.0	-1.4				
-13.5	-16.9	-0.2	-0.9	-7.2	-4.6	-6.5	60.9	-40.9	20.4	47.1	-16.1	34.7	-5.6	-2.1	-0.1	-84.5	34.0	-51.1	27.4	98.7	-63.3	-135.5				
-81.8	86.5	-178.2	-91.0	67.6	-191.7	-96.7	66.5	-145.3	-104.6	59.7	-123.2	-67.3	80.7	-198.7	-97.9	116.9	-0.8									
53.3	23.4	-6.7	13.8	9.8	-12.0	-8.5	10.8	-7.0	-7.8	13.6	-2.0	-1.0	1.9	-13.3	-33.0	6.6	-27.1	-36.9	27.9	-34.6	-31.1	30.1	0.4			
-8.5	5.4	-3.4	10.2	11.3	-20.9	-28.3	-16.8	-21.0	-26.3	-15.8	-8.0	-10.2	-13.4	-8.0	-14.0	-12.8	14.9	-0.4	-0.8	-0.3	16.4	0.7				
dicyclohexylamine 3			-1.7	-15.3	6.9	-24.8	14.0	1.2	-21.7	13.5	-15.1	-8.5	7.8	-17.9	-22.3	-11.3	-12.0	17.9	-12.0	-16.1	1.9	-4.7				
-13.2	-16.1	-1.8	-1.7	-9.6	-6.3	-7.3	59.6	-43.2	18.6	47.4	-20.2	33.3	-8.0	-2.0	1.3	-86.4	30.5	-45.1	21.7	91.7	-63.4	-131.0				
-78.3	85.3	-175.5	-89.4	71.2	-191.0	-94.7	62.6	-139.6	-99.9	55.0	-122.1	-69.0	80.6	-195.2	-97.1	116.3	-1.9	47.8								
21.1	-8.0	12.3	11.7	-14.6	-10.5	7.4	-8.4	-10.2	11.2	-2.4	-1.0	4.5	-14.2	-36.0	5.0	-28.9	-36.6	27.9	-34.0	-33.8	30.0	-2.9	-12.3			
2.2	-10.0	1.5	7.2	-18.8	-26.1	-11.2	-18.5	-24.9	-11.2	-7.2	-10.2	-9.2	-8.3	-13.9	-12.4	17.8	-5.9	-8.5	-6.4	9.6	-5.3					
dicyclohexylamine.avg			-0.6	-13.3	9.1	-24.4	15.0	2.7	-20.0	15.5	-13.1	-5.5	9.2	-14.1	-18.6	-9.1	-11.5	22.0	-11.0	-12.8	2.2	-2.8				
-13.2	-16.2	0.0	-0.9	-7.7	-4.0	-5.6	59.2	-40.0	19.7	44.2	-15.2	33.4	-5.3	-1.1	1.5	-87.4	29.9	-40.8	23.6	95.7	-61.1	-135.2				
-80.4	87.7	-178.0	-89.8	73.5	-192.5	-96.1	62.8	-142.7	-99.7	65.5	-123.6	-68.5	83.3	-198.4	-96.8	118.2	-1.6	48.7								
21.8	-6.8	13.2	10.6	-13.1	-9.0	10.2	-7.1	-8.9	13.6	-1.8	-1.2	3.2	-13.5	-34.7	5.4	-27.9	-37.7	30.1	-34.6	-33.3	31.5	-0.9	-8.7			
4.5	-4.7	7.0	8.7	-20.3	-26.9	-13.1	-20.3	-25.4	-13.2	-6.2	-8.5	-9.4	-6.5	-11.8	-11.1	11.0	-0.6	-2.2	-1.9	11.7	-0.9					
N,N-dimethylhexylamine 1			-2.7	-5.4	18.4	-4.4	28.2	11.3	-13.0	27.0	-2.0	-7.1	25.3	-8.1	8.9	28.2	33.2	25.2	14.3	17.8	27.3					
22.9	9.6	-8.6	12.4	24.3	-2.5	8.4	8.5	29.7	2.2	39.6	1.6	5.6	11.8	-2.5	18.2	25.3	-31.0	22.5	8.8	18.4	74.6	-16.8	-			
116.5	-85.4	89.3	-143.9	-85.8	46.8	-189.7	-91.9	51.8	-126.2	-96.3	80.5	-113.1	-85.0	99.6	-188.8	-99.3	107.3	-4.0								
78.1	34.0	-2.7	20.6	14.8	-10.4	-7.6	15.4	-4.7	-6.4	14.4	0.7	2.7	6.3	-5.6	-23.5	8.5	-19.0	-29.1	31.5	-24.3	24.0	23.0	-1.0			
-4.5	10.4	-2.9	6.8	4.6	-0.6	-14.3	-9.3	-1.2	-12.5	-7.2	3.8	-0.4	2.1	2.7	-1.0	-3.1	0.5	9.7	7.3	2.2	8.2	13.4				
N,N-dimethylhexylamine 2			4.1	-1.4	24.6	-2.8	30.8	16.7	-9.6	25.4	-4.6	-5.8	24.9	-8.1	4.2	21.1	17.2	26.7	12.0	10.4	23.5					
20.7	5.6	-3.5	14.4	24.1	-3.1	8.3	5.5	37.5	-7.6	29.2	4.5	4.1	12.1	-4.0	13.9	19.5	-23.0	30.2	7.8	24.0	73.6	-16.3	-			
109.5	-79.5	81.3	-141.8	-83.9	47.2	-188.1	-92.2	61.1	-119.0	-85.8	67.0	-113.1	-87.7	98.8	-196.0	-107.7	109.8									
0.9	74.3	37.4	0.1	28.6	17.9	-10.5	-6.9	19.4	-4.1	-6.3	15.4	1.7	2.7	6.7	-2.9	-20.9	5.1	-11.9	-22.1	27.2	-20.5	21.6				
-0.6	-0.7	6.7	-1.7	7.5	3.4	-4.2	-14.9	-13.3	-0.3	-10.8	-10.2	0.1	-4.0	-2.5	-7.4	-11.8	-3.2	0.2	6.7	2.6	1.3	9.0	13.2			
N,N-dimethylhexylamine 3			-0.6	-4.7	18.6	-8.1	26.9	14.2	-12.6	21.5	-6.4	-9.2	22.5	-12.2	0.2	15.4	16.1	20.0	7.8	8.8	22.7					
18.3	4.6	-9.2	8.5	23.3	-6.3	5.9	2.3	39.5	-17.5	26.4	12.8	8.2	26.5	-7.9	11.3	19.2	-30.3	24.4	3.4	11.9	62.5	-17.5	-			
114.5	-82.4	77.5	-151.9	-91.4	47.6	-192.3	-97.9	57.9	-124.6	-98.1	72.6	-117.8	-91.6	96.4	-192.6	-106.4	105.7									
-5.0	67.5	31.8	-6.7	15.0	12.5	-14.7	-10.8	10.8	-7.5	-9.5	10.3	-1.8	-0.2	1.7	-10.3	-26.0	7.0	-20.2	-29.8	25.3	-26.0	-26.1	21.5			
-0.8	-3.7	6.9	0.3	10.8	7.6	-6.6	-19.2	-15.7	-3.4	-15.6	-10.4	-1.7	-7.1	-5.4	-11.6	-14.3	-5.4	0.1	3.8	-1.5	-5.6	2.2	7.8			
N,N-dimethylhexylamine Avg			0.3	-3.8	20.6	-5.1	28.6	14.0	-11.7	24.6	-4.3	-7.4	24.2	-9.4	4.4	21.6	22.2	24.0	11.4	12.4	24.5					
20.6	6.6	-7.1	11.8	23.9	-3.9	7.5	5.4	35.6	-7.6	31.7	6.3	5.9	16.8	-4.8	14.5	21.3	-28.1	25.7	6.7	18.1	70.2	-16.8	-			
113.5	-82.4	82.7	-145.9	-87.0	47.2	-190.0	-94.0	56.9	-123.2	-93.4	73.4	-114.7	-88.1	98.3	-192.5	-104.5	107.6									
-2.7	73.3	34.4	-3.1	21.4	15.1	-11.9	-8.4	15.2	-5.5	-7.4	13.4	0.2	1.7	4.9	-6.2	-23.5	6.9	-17.0	-27.0	28.0	-23.6	22.0				
-0.8	-3.0	8.0	1.5	8.3	5.2	-3.8	-16.1	-12.8	-1.7	-13.0	-9.3	0.7	-3.8	-1.9	-5.5	-9.0	-3.9	0.3	6.8	2.8	-0.7	6.5	11.5			
3,4-Lutidine 1			-5.6	-20.7	9.8	-39.1	11.0	-27.0	-23.7	8.3	-22.3	-6.9	4.7	-16.4	-0.3	-3.5	0.9	53.5	1.5	21.0	4.5	-3.1	-7.9			
-24.2	-8.7	-16.4	-15.3	-4.3	-10.0	64.3	-31.4	37.7	67.6	-14.0	13.2	8.2	7.7	10.5	-6.5	105.5	-90.3	43.6	115.5	-76.0	-137.3	-				
102.3	45.4	-3.4	13.7	-15.0	-37.9	-11.2	2.3	-114.8	-72.9	-19.6	-131.3	-90.2	81.3	-161.0	-94.7	28.8	-0.3	29.4	6.4	1.2						
0.7	7.5	-9.4	-0.2	-5.6	-13.2	-9.6	-19.9	-0.4	4.6	6.5	-1.0	5.2	6.1	1.8	14.3	5.8	2.3	7.7	5.4	-2.5	-14.7	5.4	-18.5			
9.5	-5.7	-11.2	2.1	1.2	-3.4	10.2	7.2	-7.4	-14.5	6.5	-11.8	-15.1	2.5	24.7	-14.5	-17.2	-4.8	22.8	1.1							
3,4-Lutidine 3			0.3	-7.5	16.2	-25.8	24.0	-17.4	-18.7	13.9	-12.3</td															

2-picoline 1	-7.6	-19.9	9.7	-31.6	8.7	-15.4	-29.3	-2.5	-17.7	-21.4	-10.1	-19.2	-19.4	-3.0	-4.7	11.9	-9.1	-9.9	5.4	-0.5	-3.9	-30.6		
	-10.7	-19.3	-16.6	-11.9	-12.8	65.8	-11.7	22.0	62.1	-12.8	6.0	-11.2	-6.7	0.9	-2.5	103.2	-98.1	37.0	115.3	-86.7	-140.8	-107.8		
	51.3	-4.3	6.0	-33.7	-42.2	-8.2	11.5	-111.7	-75.3	-20.0	-145.7	-105.5	68.4	-172.2	-95.9	45.1	0.1	21.0	-5.4	0.2				
	2.0	2.3	-1.7	0.6	1.6	-1.3	3.9	0.3	-3.9	3.8	1.2	0.7	-13.8	5.8	-7.7	-7.8	7.6	-12.6	-10.9	9.7	0.4			
	11.6	7.3	8.1	11.9	6.1	9.7	12.8	5.1	4.0	-1.5	0.2	-0.6	-3.0	-0.6	28.6	0.3	3.3	0.6	31.8	5.8				
2-picoline 2	2.4	-17.2	16.4	-25.3	16.0	-9.2	-25.6	8.7	-16.1	-16.8	-11.0	-19.1	-14.3	0.3	-2.9	16.2	-4.7	-7.8	2.5	-1.4	-3.9	-24.7		
	-5.8	-17.2	-11.6	-9.7	-8.7	68.8	-18.2	19.1	63.4	-15.5	3.9	-3.6	-2.8	0.9	0.7	108.5	-95.9	41.2	115.7	-77.2	-137.7	-103.3		
	44.1	-1.4	10.2	-30.8	-31.3	-6.2	7.7	-108.3	-73.3	-37.2	-144.6	-107.2	71.5	-167.8	-96.5	32.6	-0.5	30.6	4.1	-0.7				
	12.2	4.3	2.1	1.8	5.6	-2.5	4.3	0.2	-0.1	2.4	4.3	-0.3	-7.7	3.6	3.4	-4.5	11.4	-8.1	-7.0	11.3	1.0	3.2		
	1.7	-0.6	3.3	3.9	2.1	2.1	4.6	3.7	0.4	0.5	3.1	0.0	1.3	1.8	32.0	-3.8	-2.4	0.4	30.6	5.2				
2-picoline 3	6.2	-10.2	21.8	-22.3	20.1	-4.9	-17.5	15.7	-5.6	-5.3	-1.0	-9.8	-7.2	7.6	-0.4	19.7	0.3	-2.4	5.4	1.6	-1.5	-15.3		
	1.6	-12.5	-2.8	-2.3	-1.1	70.8	-15.3	25.4	64.7	-13.6	7.0	3.4	2.8	4.7	1.0	105.7	-95.2	46.1	110.7	-72.2	-136.6	-98.9		
	-0.3	9.6	-28.8	-27.4	-5.7	2.4	-109.4	-69.2	-35.6	-140.0	-97.8	66.6	-170.9	-94.6	32.5	0.5	26.6	4.5	1.3	9.0	7.3			
	2.3	2.2	7.9	0.2	4.4	-0.1	-2.7	1.7	3.6	2.0	-8.0	5.4	1.0	-2.3	10.2	-9.3	-5.9	9.9	-0.5	5.1	3.6	2.8		
	0.6	2.0	0.6	3.4	3.7	4.6	1.9	-2.3	3.8	4.1	-0.1	2.6	33.7	-3.1	-1.2	1.5	28.7	6.0						
Avg 2-picoline	0.3	-15.8	16.0	-26.4	14.9	-9.8	-24.1	7.3	-13.2	-14.5	-7.3	-16.0	-13.6	1.6	-2.6	15.9	-4.5	-6.7	4.4	-0.1	-3.1			
	-23.5	-5.0	-16.3	-10.3	-7.9	-7.5	68.5	-15.1	22.1	63.4	-14.0	5.6	-3.8	-2.2	2.2	-0.3	105.8	-96.4	41.4	113.9	-78.7	-138.4	-	
	103.3	47.6	-2.0	8.6	-31.1	-33.7	-6.7	7.2	-109.8	-72.6	-30.9	-143.4	-103.5	68.8	-170.3	-95.7	36.8	0.0	26.1	1.1				
	0.3	7.8	4.6	0.9	1.5	5.0	-1.2	4.2	0.2	-2.2	2.6	3.1	0.8	-9.8	4.9	-1.1	-4.9	9.7	-10.0	-7.9	10.3	0.3		
	-0.6	5.3	2.9	4.0	5.9	2.9	5.1	7.1	4.5	2.1	-1.1	2.4	1.1	-0.6	1.3	31.4	-2.2	-0.1	0.8	30.4	5.7			
3-picoline 1	1.6	-10.5	17.8	-26.9	23.5	-9.5	-16.5	17.4	-5.2	-7.3	8.3	-7.9	-6.2	0.4	3.0	69.9	1.1	30.9	10.4	5.1	-1.9	-16.9		
	1.0	-10.7	-8.4	-0.1	-8.0	73.3	-14.0	31.0	60.7	-6.9	6.8	0.3	5.0	4.4	0.1	116.4	-93.3	38.0	124.1	-84.6	-143.2	-105.5		
	50.6	-0.1	10.6	-30.1	-23.7	-5.4	5.5	-108.3	-70.1	-24.2	-147.5	-108.9	74.3	-161.9	-84.1	37.0	-0.1	20.6	-3.7	1.0				
	3.8	2.4	-0.3	1.8	-0.2	1.3	4.9	-1.1	-5.9	-0.7	-0.5	-1.9	-10.7	2.9	-3.7	1.8	4.6	-3.1	-3.4	6.9	-0.2	3.8	7.9	
	10.1	1.3	16.0	22.2	8.0	21.0	23.8	9.3	0.1	-1.9	7.6	0.3	2.0	11.5	27.8	0.9	-0.2	0.2	33.4	5.9				
3-picoline 2	5.6	-10.7	20.8	-29.8	22.2	-10.2	-24.7	9.9	-14.6	-18.5	1.9	-16.9	-8.2	0.5	4.2	57.2	-1.1	25.7	9.2	3.6	-6.1	-22.6		
	-2.3	-12.5	-11.4	-5.0	-13.5	71.0	-12.6	26.4	60.6	-10.5	7.4	-4.9	-0.8	3.5	0.7	111.3	-94.4	43.4	121.1	-85.2	-143.0	-108.9		
	42.6	-2.6	10.8	-23.7	-30.5	-6.1	9.0	-107.8	-67.5	-24.4	-146.3	-103.8	67.4	-164.0	-83.6	31.9	-1.1	23.8	0.1	0.0				
	5.6	1.3	3.5	3.9	5.2	-0.5	6.6	-0.6	-0.5	2.7	3.9	1.5	-7.0	10.9	3.6	2.6	12.9	-4.2	-3.3	12.4	0.2	7.5	8.4	
	11.8	2.0	12.2	15.7	9.1	15.8	20.7	8.8	-0.2	-2.5	4.5	-1.2	6.9	9.4	32.3	5.6	5.1	0.6	38.5	10.7				
3-picoline3	3.0	-9.2	19.3	-29.3	23.1	-9.4	-18.7	11.5	-13.1	-14.4	8.1	-14.9	-9.2	-0.4	-0.3	56.9	0.0	26.4	10.8	4.8	-1.8	-19.5		
	-1.0	-8.4	-9.1	-3.4	-6.2	69.0	-14.1	24.1	60.4	-13.3	8.5	0.8	0.1	5.9	0.8	110.8	-92.0	42.3	118.5	-82.7	-138.5	-103.4		
	47.1	-1.1	10.6	-24.0	-26.8	-7.2	6.9	-107.0	-69.6	-24.6	-129.0	-92.4	64.0	-160.5	-78.0	36.7	0.4	22.9	-1.8	0.7	9.9			
	7.1	7.1	6.4	8.9	0.9	8.9	1.8	-2.8	4.5	4.6	0.1	-2.0	7.2	7.6	9.7	11.5	2.1	1.3	13.6	-1.3	11.2	10.8	0.2	
	0.8	16.0	23.1	7.7	20.4	24.9	10.8	-0.5	0.0	3.6	0.7	2.2	11.0	29.8	-0.8	3.9	0.2	28.1	3.1					
Avg 3-picoline	3.4	-10.2	19.3	-28.6	22.9	-9.7	-20.0	12.9	-11.0	-13.4	6.1	-13.2	-7.9	0.2	2.3	61.3	0.0	27.7	10.1	4.5	-3.2			
	-19.7	-0.8	-10.5	-9.6	-2.8	-9.2	71.1	-13.6	27.2	60.6	-10.2	7.6	-1.3	1.5	4.6	0.5	112.9	-93.2	41.2	121.3	-84.2	-141.6	-	
	105.9	46.7	-1.3	10.7	-25.9	-27.0	-6.2	7.1	-107.7	-69.1	-24.4	-141.0	-101.7	68.6	-162.1	-81.9	35.2	-0.3	22.5	-1.8				
	0.6	6.4	3.6	3.4	4.1	4.6	0.6	6.8	0.0	-3.1	2.2	2.7	-0.1	-6.6	7.0	2.5	4.7	9.6	-1.7	-1.8	11.0	0.4	7.5	9.0
	0.5	11.2	1.4	14.7	20.3	8.3	19.1	23.1	9.6	-0.2	-1.5	5.2	-0.1	3.7	10.6	29.9	1.9	2.9	0.4	33.3	6.6			
4-picoline 1	3.8	-10.8	20.3	-22.2	21.6	-11.5	-25.4	7.3	-11.4	-14.7	2.7	-12.1	-6.1	-1.1	5.4	57.9	0.9	33.9	13.5	4.7	1.6	-17.0		
	1.0	-6.3	-10.0	8.0	3.1	61.6	-20.7	30.4	56.2	-2.9	19.8	4.1	4.6	10.2	-6.0	101.5	-72.8	40.4	112.8	-65.9	-131.5	-86.7		
	-6.7	15.5	-2.5	-48.9	-0.7	14.5	-101.8	-52.8	2.5	-132.9	-88.0	78.8	-164.9	-75.2	54.4	3.4	29.9	12.1	-3.8	5.8	5.9			
	1.9	6.6	6.0	-0.1	8.5	4.5	-3.4	0.9	2.0	1.4	-1.8	3.2	3.4	9.0	7.2	-1.1	4.1	10.5	1.8	6.7	11.5	-4.1	18.9	4.3
	16.0	26.5	8.2	19.6	32.3	8.3	0.8	1.3	13.0	2.4	-5.9	5.7	38.1	-1.1	3.3	3.8	18.5	-4.3						
4-picoline 2	-0.2	-16.5	14.9	-28.8	16.7	-13.8	-24.1	8.8	-12.0	-11.9	1.2	-14.4	-4.4	-3.7	5.6	52.5	-0.9	31.8	13.8	6.9	2.3	-18.4		
	2.4	-5.4	9.2	1.9	3.0	67.2	-17.0	31.7	57.4	-2.9	16.6	-5.3	1.6	2.4	-1.3	111.7	-79.0	46.8	125.4	-66.5	-135.0	-93.5		
	-5.0	14.2	-6.3	-45.0	0.7	14.2	-104.7	-58.7	-1.2	-138.7	-93.6	78.8	-170.1	-80.8	56.7	-0.6	31.7	9.4	-1.1	6.0	5.9			
	3.6	6.3	3.5	-1.5	7.5	0.2	-5.1	1.7	5.5	-1.9	-3.0	5.3	4.5	9.8	5.2	-0.7	2.6	9.1	-0.3	5.2	10.0	-2.3	21.0	8.7
	24.8	35.4	14.7	29.6	42.7	16.8	3.7	2.2	15.3	3.2	-2.8	7.7	36.3	0.9	3.2	1.1	13.3	-10.7						
4-picoline 3	1.3	-8.7	20.5	-18.0	25.7	-6.4	-9.9	23.6	1.2	-8.3	9.9	-10.0	-9.1	-4.4	3.5	54.7	-5.4	28.8	13.2	4.9	1.7	-12.3		
	2.0	-4.5	1.4	12.5	17.8	78.6	-8.7	41.2	56.3	-2.4	20.9	-7.5	-3.5	2.2	-4.2	100.8	-81.1	35.2	113.1	-74.3	-137.7	-94.1		
	0.8	26.5	-0.4	-43.4	-3.1	16.4	-103.2	-64.1	-7.1	-141.7	-92.9	89.6	-176.4	-88.4	48.1	0.1	24.1	5.0	0.1	10.3	6.4			
	2.7	5.4	6.0	-0.1	4.8	-2.4	-1.2	6.0	5.8	0.3	-1.4	5.0	-4.4	3.9	-0.8	-0.8	6.4	2.2	1.1	4.8	12.7	-0.1	20.7	5.5
	14.0	26.0	6.7	34.6	46.4	18.5	1.4	0.4	16.9	-1.6	-9.0	-3.6	30.0	2.7	6.5	-0.3	23.5	-3.1						
Avg 4-picoline	1.6	-12.0	18.6	-23.0	21.3	-10.6	-19.8	13.2	-7.4	-11.7	4.6	-12.1	-6.5	-3.0	4.8	55.0	-1.8	31.5	13.5	5.5	1.9			
	-15.9	1.8	-5.4	-6.0	5.1	8.0	69.2	-15.5	34.5	56.6	-2.7	19.1												

31.6	-2.9	7.8	-23.0	-10.0	-7.2	2.2	-87.7	-54.9	-31.7	-125.4	-86.2	49.7	-123.5	-60.1	17.0	0.0	20.5	-3.2	-2.7	4.4	0.3			
-5.0	-2.2	1.3	-4.1	1.8	-2.3	0.7	1.0	4.5	-0.1	-11.1	4.5	-2.3	-7.8	10.8	-14.8	-14.5	12.7	0.0	1.9	4.4	0.0			
4.6	4.8	4.2	5.0	6.1	5.4	0.1	7.9	8.2	0.2	7.1	7.5	25.6	3.3	3.6	0.9	32.9	7.6				2.2	2.4		
decylamine 1			3.4	-34.5	26.9	-40.1	23.2	-19.7	-35.8	11.2	-29.1	-17.0	-13.9	-26.9	10.7	-13.5	7.6	42.9	-13.0	19.8	3.6	-0.4	-9.4	
-19.1	1.6	-4.9	-24.1	-6.0	2.4	63.3	-35.6	-18.4	51.7	-14.1	19.4	-10.0	-2.8	1.6	-114.2	-5.0	-31.1	-25.9	63.0	-50.7	-108.1			
-75.3	56.8	-158.7		-80.5	72.7	-180.8		-87.5	109.1	-115.7		-93.9	37.5	-144.0		-100.7		102.6	-184.7		-95.8	108.4	0.2	
87.3	32.0	0.0	39.1	20.9	1.5	3.2	10.6	2.2	0.0	13.7	-13.9	-4.9	5.9	-2.3	-59.9	12.4	-35.1	-49.5	55.5	-53.8	-50.6	64.3	1.3	
-6.5	10.9	0.5	33.0	24.0	-36.3	-40.3	-25.8	-16.7	-21.2	-13.9	-0.5	-4.0	2.7	-3.5	-3.6	3.4	28.8	1.9	-2.0	-0.1	15.2	0.6		
decylamine 2			9.5	-17.4	27.1	-34.7	27.4	-13.8	-21.8	16.9	-19.7	-5.6	-0.3	-18.4	-13.9	-7.7	-4.1	46.0	-11.2	21.8	1.0	-1.8	-6.7	
-16.2	5.5	-0.7	-18.4	-2.7	7.4	71.3	-29.9	-6.6	53.9	-10.0	25.3	-8.7	-3.5	2.4	-87.4	30.7	-50.9	-25.3	66.2	-53.3	-121.3		-82.6	
67.3	-169.7		-82.7	65.2	-192.1		-91.9	107.5	-125.2		-101.0		38.2	-151.7		-106.0		94.2	-195.3		-102.8		106.0	
0.4	87.6	31.1	-0.8	37.4	21.8	-6.3	-3.0	7.7	-2.2	-4.0	9.6	-17.1	-9.6	2.9	-17.3	-64.0	7.6	-40.4	-56.8	50.2	-56.8	-54.4	58.6	
-1.5	-11.6	5.7	-2.4	29.6	23.9	-34.6	-39.6	-23.6	-19.1	-24.7	-14.4	-4.0	-8.1	-0.5	-8.9	-7.4	-0.6	34.1	0.4	-3.0	0.5	14.0	2.3	
decylamine 3			0.6	-17.5	23.8	-42.6	21.0	-17.4	-37.2	9.3	-32.0	-16.6	-7.5	-28.9	6.7	-12.8	6.1	42.6	-13.3	21.0	2.8	-1.0	-9.3	
-21.7	2.0	-4.6	-23.6	-7.6	1.1	64.9	-30.0	-9.7	49.5	-17.1	18.4	-5.1	-1.9	3.0	-116.9	-3.2	-34.8	-26.0	63.6	-51.3	-114.7			
-78.0	59.0	-161.9		-78.6	66.1	-184.4		-88.7	109.0	-114.2		-95.2	30.0	-146.2		-101.8		98.7	-187.7		-98.3	107.9	0.6	
87.0	34.1	-3.9	35.3	26.4	-1.0	-0.2	5.7	1.6	-0.6	11.1	-14.9	-4.3	4.3	-14.2	-59.7	8.3	-35.2	-49.5	48.3	-53.7	-51.7	62.3	-0.3	
-5.3	11.9	-0.3	32.9	30.4	-31.9	-37.4	-23.4	-14.8	-22.8	-12.1	1.3	-3.6	1.0	-3.6	-3.4	0.7	33.6	1.2	-2.7	-0.2	19.3	3.3		
Avg decylamine			4.5	-23.1	25.9	-39.2	23.9	-17.0	-31.6	12.5	-27.0	-13.1	-7.2	-24.7	1.2	-11.4	3.2	43.8	-12.5	20.8	2.4	-1.1	-8.5	
-19.0	3.0	-3.4	-22.0	-5.4	3.7	66.5	-31.8	-11.6	51.7	-13.7	21.1	-7.9	-2.8	2.3	-106.2	7.5	-38.9	-25.8	64.2	-51.8	-114.7			
-78.6	61.0	-163.4		-80.6	68.0	-185.8		-89.3	108.5	-118.4		-96.7	35.2	-147.3		-102.8		98.5	-189.2		-98.9	107.4	0.4	
87.3	32.4	-1.5	37.3	23.1	-1.9	0.0	8.0	0.6	-1.5	11.4	-15.3	-6.3	4.4	-11.3	-61.2	9.4	-36.9	-51.9	51.3	-54.8	-52.2	61.8	-0.2	
-7.8	9.5	-0.7	31.8	26.1	-34.3	-39.1	-24.3	-16.8	-22.9	-13.5	-1.1	-5.2	1.1	-5.3	-4.8	1.2	32.1	1.2	-2.6	0.1	16.2	2.1		
1-Pentylthiol 1			-5.2	-3.5	-2.5	-0.1	-3.2	9.8	-8.2	-7.7	-7.2	-41.1	-2.4	-5.7	2.9	6.8	4.5	28.2	52.2	79.6	11.7	8.0	38.9	
-2.2	-4.2	3.8	-9.3	-1.8	21.3	11.8	0.8	-18.2	9.8	4.5	4.5	2.1	2.0	0.9	2.5	12.1	8.7	4.7	4.5	4.5	0.0	0.3	9.6	
-0.7	4.5	7.4	-0.4	1.4	5.7	1.1	5.3	6.0	1.2	4.2	6.9	-0.3	7.5	5.9	0.4	9.9	13.9	-0.1	9.4	8.0	-0.6	3.0	0.4	
2.2	3.1	-1.2	0.3	0.5	2.6	3.4	-0.1	5.7	3.3	4.6	9.5	0.7	-0.1	6.4	0.4	2.6	5.4	0.9	1.3	-2.6	-3.0	-1.0	2.2	
48.0	42.3	32.2	1.6	2.3	7.6	7.3	9.2	10.0	-0.3	14.1	8.6	0.8	5.1	10.7										
1-Pentylthiol 2			1.3	0.3	0.5	2.7	-7.1	11.9	-9.8	-7.5	-7.3	-46.5	-2.6	-11.7	0.0	2.2	1.1	31.9	54.9	82.1	7.7	4.1	32.3	
-2.1	-2.5	3.5	-7.8	0.9	18.3	10.4	1.9	-13.9	3.9	1.2	-1.7	-2.8	0.2	3.2	-0.1	7.4	4.7	1.7	4.5	3.2	0.2	1.2	6.4	
-1.5	4.1	9.0	-0.8	-0.1	3.7	-0.2	1.7	4.1	1.8	2.9	7.9	-0.6	5.8	4.9	1.6	7.4	11.2	0.0	9.3	7.6	3.6	5.2	0.9	
1.5	3.4	0.8	0.2	0.5	3.4	2.3	-3.7	2.4	2.4	1.8	5.5	-1.8	-1.1	8.4	-0.3	4.3	5.9	1.7	4.1	-0.5	-2.8	4.2		
42.4	34.4	26.6	3.2	2.6	5.4	7.7	7.6	10.3	0.3	12.2	6.4	1.2	9.2	16.0										
1-Pentylthiol 3			-0.5	0.5	1.3	6.5	-10.0	16.2	-7.7	-4.1	-4.8	-43.6	-2.0	-6.8	-8.1	-4.1	-0.1	10.8	34.5	60.1	6.1	4.8	24.9	
1.4	0.0	8.1	-5.1	2.3	15.0	7.9	0.7	-16.6	3.5	0.4	0.3	2.0	1.5	2.5	1.1	6.9	5.4	6.2	4.0	4.4	0.3	2.8	8.0	
2.2	7.1	9.5	0.2	4.7	3.0	0.7	6.7	5.6	0.5	0.7	3.5	-0.3	3.0	1.9	-0.3	4.3	4.2	-0.3	12.3	5.7	2.1	3.5	5.3	
1.7	2.8	2.4	-1.0	-0.5	0.4	0.0	-5.3	1.0	0.3	-2.0	4.4	-4.3	-4.7	3.6	0.0	1.7	2.5	1.4	1.8	-0.3	-1.3	-1.0	0.9	
31.5	27.1	21.2	1.3	0.3	1.7	-0.8	3.4	3.7	0.0	4.8	2.8	-1.0	4.9	7.1										
Avg 1-Pentylthiol			-1.5	-0.9	-0.2	3.1	-6.8	12.7	-8.5	-6.4	-6.5	-43.7	-2.3	-8.1	-1.7	1.7	1.8	23.6	47.2	73.9	8.5	5.6	32.0	
-1.0	-2.2	5.1	-7.4	0.5	18.2	10.0	1.1	-16.2	5.7	2.0	1.0	0.4	1.2	2.2	1.2	8.8	6.3	4.2	4.3	4.0	0.2	1.4	8.0	
0.0	5.3	8.7	-0.3	2.0	4.1	0.5	4.6	5.2	1.2	2.6	6.1	-0.4	5.4	4.3	0.5	7.2	9.8	-0.1	10.3	7.1	1.7	3.9	2.2	
1.8	3.1	0.7	-0.2	0.2	2.1	1.9	-3.0	3.0	2.0	1.5	6.5	-1.8	-2.0	6.1	0.1	2.9	4.6	1.3	2.4	-1.1	-2.4	-1.6	2.4	
40.7	34.6	26.7	2.0	1.7	4.9	4.8	6.8	8.0	0.0	10.3	6.0	0.3	6.4	11.3										
1-Hexylthiol 1			-0.2	0.9	0.1	5.4	-7.7	16.6	-7.9	-5.3	-3.7	-32.7	-0.7	-8.0	-9.0	-2.7	-0.3	12.5	37.6	58.9	3.1	2.6	11.5	
-3.3	-1.4	5.6	-7.7	-3.3	10.7	-0.1	-3.9	-9.5	1.5	-2.2	-1.8	-5.1	-0.8	-0.3	1.4	2.0	0.1	-1.4	2.5	-0.9	-0.6	-3.7	-0.1	
-3.2	-2.5	-1.2	-2.0	-3.4	2.0	-3.2	-3.7	1.4	2.9	1.8	3.5	0.1	0.7	0.9	0.4	2.0	4.5	-0.8	0.0	0.8	0.3	1.1	-2.1	
1.5	1.8	-3.1	0.9	1.9	2.4	2.5	0.1	2.8	1.7	1.1	2.4	1.4	-0.4	5.5	0.3	4.1	2.8	3.3	0.4	1.0	-0.3	1.4	3.4	
20.5	17.8	18.6	2.1	5.4	4.2	6.9	7.1	6.2	0.1	7.0	5.3	2.3	5.3	5.6										
1-Hexylthiol 2			-1.7	-4.5	-2.3	3.5	-8.0	11.2	-5.8	-6.0	-5.5	-35.4	1.8	-0.4	-5.4	-2.6	-2.4	28.7	53.8	74.3	11.2	6.2	40.1	
-7.0	-7.8	-0.2	-9.6	-0.3	16.7	10.3	1.3	-17.3	4.9	2.6	1.2	-1.1	-1.2	-0.4	-6.0	3.2	-2.2	-1.1	3.2	-1.2	0.1	-1.5	0.7	
0.3	2.8	7.3	0.2	2.8	5.3	1.0	5.1	5.6	0.4	-0.8	4.3	-0.7	0.7	3.7	-1.5	5.7	7.7	0.8	1.9	8.0	3.4	3.4	2.9	
3.3	6.6	3.8	3.3	4.2	2.8	4.8	2.7	2.8	2.2	3.3	2.4	5.6	6.9	4.7	2.8	5.1	3.2	5.6	4.6	-1.5	6.9	8.7	8.1	
49.7	41.5	32.6	4.7	5.5	6.5	3.0	3.3	2.6	1.4	6.9	3.4	5.2	4.9	8.0										
Avg 1-Hexylthiol			-0.9	-1.8	-1.1	4.5	-7.8	13.9	-6.8	-5.7	-4.6	-34.1	0.6	-4.2	-7.2	-2.7	-1.4	20.6	45.7	66.6	7.2	4.4	25.8	
-5.2	-4.6	2.7	-8.6	-1.8	13.7	5.1	-1.3	-13.4	3.2	0.2	-0.3	-3.1	-1.0	-0.4	-2.3	2.6	-1.1	-1.3	2.8	-1.0	-0.3	-2.6	0.3	
-1.4	0.1	3.1	-0.9	-0.3	3.6	-1.1	0.7	3.5	1.7	0.5	3.9	-0.3	0.7	2.3	-0.5	3.9	6.1	0.						

4.9	32.7	31.0	14.8	-1.9	-4.7	2.6	5.9	8.5	6.9	0.7	5.7	3.2	0.7	1.4	5.5
cyclohexylthiol 1															
0.3	-0.9	2.8	-7.0	3.9	13.9	2.9	0.9	-5.2	2.5	0.6	0.1	-1.9	0.4	-1.7	0.5
0.1	4.1	5.2	0.2	1.4	1.5	0.1	6.0	10.2	2.6	5.9	4.0	-0.1	2.7	4.6	0.2
1.2	3.4	0.5	1.2	1.4	4.5	3.4	2.9	2.7	0.7	2.6	2.3	2.6	2.9	1.4	0.0
39.8	33.8	25.9	-0.4	-1.3	3.3	-0.2	-2.6	-1.0	-1.1	2.4	-0.2	0.3	-0.4	-4.5	
cyclohexylthiol 2															
-1.8	-2.1	4.9	-9.9	-1.9	10.4	1.3	-0.3	-7.0	3.9	-1.3	0.6	-1.6	0.4	1.0	0.3
-0.3	4.5	8.8	-0.4	0.0	4.2	0.0	4.5	10.9	2.0	5.0	8.7	-1.4	8.1	7.8	0.6
3.1	6.4	2.7	4.2	3.8	4.0	3.4	5.2	4.5	3.9	6.1	5.9	5.0	5.8	5.4	0.3
26.0	22.2	16.8	0.0	-0.5	3.9	-1.6	-0.8	2.5	0.4	10.0	6.0	0.4	2.4	2.2	
cyclohexylthiol 3															
0.2	-0.8	3.2	-2.7	0.6	16.8	1.3	1.3	-4.7	2.4	0.6	0.6	-0.8	0.5	-1.1	0.3
0.0	4.5	5.7	0.8	1.4	0.6	0.6	5.0	11.7	0.9	2.0	8.9	0.2	3.6	2.3	1.7
1.1	3.7	-0.5	-0.4	0.5	1.6	0.9	2.5	0.8	0.4	2.5	4.0	1.0	2.6	1.5	-0.2
31.8	27.5	19.5	-0.8	-1.7	1.5	-3.9	-4.2	0.5	-1.8	3.3	1.7	0.3	0.7	-1.9	
Avg cyclohexylthiol															
-0.6	-0.6	-0.2	2.4	-2.9	15.8	-3.1	-4.8	-2.1	-20.8	-1.3	-5.9	-6.8	-2.7	-0.3	24.7
3.2	-0.4	-1.3	3.6	-6.6	0.9	13.7	1.9	0.6	-5.7	2.9	0.0	0.4	-1.4	0.4	-0.6
11.0	-0.1	4.4	6.6	0.2	1.0	2.1	0.2	5.2	10.9	1.8	4.3	7.2	-0.4	4.8	4.9
2.2	1.8	4.5	0.9	1.6	1.9	3.4	2.5	3.5	2.7	1.7	3.7	4.1	2.9	3.7	2.8
4.2	32.5	27.8	20.7	-0.4	-1.2	2.9	-1.9	-2.6	0.6	-0.8	5.2	2.5	0.3	0.9	-1.4
3-decanone 3															
-1.3	-1.2	0.5	-2.5	-0.3	1.1	-1.7	0.6	1.5	-0.8	-15.1	1.5	0.2	3.0	3.0	-2.0
-0.1	0.4	2.7	-0.4	-1.2	5.6	-0.7	-0.6	-0.3	-1.7	0.3	2.1	-3.7	-0.6	3.8	8.7
-4.9	-1.4	2.1	-8.2	-4.7	1.0	-7.6	-4.6	-3.6	3.9	5.1	7.4	2.3	4.7	8.6	0.7
8.2	13.5	-17.5	10.2	10.9	-2.6	4.4	48.8	1.8	29.7	65.4	-12.4	47.0	55.4	-8.9	0.1
38.4	28.4	10.4	6.0	9.5	11.1	9.1	11.5	3.8	3.4	8.6	4.2	0.0	7.2	10.5	
3-decanone 1															
0.7	0.0	0.4	1.4	0.2	3.0	2.1	-0.1	1.9	-0.2	0.3	-11.0	2.3	0.8	1.5	1.4
1.3	1.5	2.5	3.0	1.2	5.3	0.0	-1.8	-0.8	1.5	1.8	1.4	3.5	2.2	4.6	0.0
0.0	4.0	5.6	0.0	3.4	3.0	1.0	2.9	1.4	1.8	3.7	8.7	0.0	5.1	4.9	0.0
9.1	12.5	-18.8	12.8	15.4	6.7	2.6	51.0	0.2	30.4	69.2	-19.5	49.7	56.3	-12.0	0.1
29.7	14.0	0.7	-13.3	-5.2	-3.1	1.4	20.3	7.3	-6.9	33.7	-0.8	-11.8	13.0	30.7	
3-decanone 2															
0.9	0.7	1.1	-0.8	4.0	2.5	1.6	4.8	0.9	1.8	-15.0	6.3	0.9	3.1	1.9	-1.6
2.0	1.7	1.8	2.5	0.1	5.0	-0.8	-1.2	-1.0	0.1	1.4	2.4	1.7	2.7	5.2	0.1
0.5	2.8	4.5	-0.1	2.8	2.0	0.2	0.6	-2.7	0.5	0.6	2.0	0.0	3.8	4.2	0.1
8.0	12.6	-26.2	8.5	8.6	-3.2	3.0	56.4	0.7	32.4	73.9	-19.6	52.1	60.0	-12.9	-0.1
48.3	30.0	12.7	-1.9	0.1	-1.4	3.2	3.4	-9.6	-4.0	-0.3	-9.9	-4.7	-0.8	0.7	
Avg 3-decanone															
0.1	-0.2	1.0	-1.0	2.2	1.9	-0.1	2.4	0.8	0.4	-13.7	3.3	0.6	2.5	2.1	-0.9
1.1	1.2	2.3	1.7	0.0	5.3	-0.5	-1.2	-0.7	0.0	1.1	1.9	0.5	1.4	4.5	2.9
-1.4	1.8	4.1	-2.8	0.5	2.0	-2.1	-0.4	-1.6	2.1	3.2	6.0	0.8	4.5	5.9	0.3
8.4	12.9	-20.8	10.5	11.6	0.3	3.3	52.0	0.9	30.9	69.5	-17.2	49.6	57.2	-11.3	0.0
38.8	24.1	8.0	-3.1	1.5	2.2	4.6	11.7	0.5	-2.5	14.0	-2.2	-5.5	6.4	13.9	
3-heptanone 1															
-8.4	-9.6	-8.5	-10.4	-2.6	-2.2	-13.3	0.3	-6.9	-2.4	-0.9	5.6	5.7	9.9	10.3	3.1
-11.3	-4.4	0.2	-7.3	-10.0	2.8	-0.1	-7.2	3.4	1.1	3.1	2.0	3.6	6.3	11.8	0.0
-4.0	2.4	10.4	-0.1	3.6	0.0	0.1	5.8	10.4	-1.6	1.0	9.2	0.0	7.2	8.0	-1.5
10.8	15.9	-26.2	17.1	17.2	6.3	2.3	71.9	8.0	34.9	88.3	-16.2	55.5	67.1	-12.6	-0.4
79.9	65.1	43.4	3.5	22.3	27.5	23.0	22.6	18.7	11.3	8.8	-1.5	-0.5	4.0	4.0	
3-heptanone 3															
-3.7	-4.9	-2.3	-6.2	1.7	5.8	-14.4	1.5	-5.4	-9.2	-4.8	2.8	2.5	20.2	38.5	7.6
-9.2	-1.7	3.3	-6.0	-5.5	8.3	-4.0	-9.7	0.0	-4.9	-1.4	-0.5	2.2	8.0	16.2	-0.5
-7.2	2.0	9.8	-0.7	0.6	1.8	-2.7	3.6	8.5	5.6	9.6	15.1	0.1	12.3	10.9	0.3
13.9	21.3	-21.1	16.4	16.3	6.4	7.1	69.0	12.1	37.4	91.1	-7.9	59.4	76.7	-3.0	0.3
63.1	57.7	31.0	6.4	21.5	27.0	14.6	15.8	24.4	13.5	14.4	9.2	2.2	7.8	8.9	
Avg 3-heptanone															
-6.0	-7.2	-5.4	-8.3	-0.4	1.8	-13.9	0.9	-6.2	-5.8	-2.9	4.2	4.1	15.1	24.4	5.4
-10.2	-3.1	1.7	-6.7	-7.7	5.5	-2.0	-8.5	1.7	-1.9	0.9	0.8	2.9	7.1	14.0	-0.2
-5.6	2.2	10.1	-0.4	2.1	0.9	-1.3	4.7	9.5	2.0	5.3	12.1	0.0	9.8	9.5	-0.6
12.3	18.6	-23.7	16.7	16.7	6.3	4.7	70.4	10.1	36.1	89.7	-12.0	57.5	71.9	-7.8	-0.1
71.5	61.4	37.2	5.0	21.9	27.2	18.8	19.2	21.6	12.4	11.6	3.9	0.8	5.9	6.5	
2-octanone 2															
9.6	10.1	9.4	12.7	17.4	15.3	2.6	9.2	2.9	2.9	-6.9	21.4	8.1	25.5	46.1	12.7
0.8	7.3	7.4	5.9	5.8	11.8	2.6	-0.3	6.3	7.1	9.9	8.2	7.8	14.4	21.6	-0.5
0.8	4.3	6.7	0.4	5.0	1.0	-0.1	6.3	2.6	-0.8	0.5	3.9	-0.1	4.5	2.7	0.4
5.8	8.7	-9.1	4.9	5.0	1.9	1.0	40.6	5.1	20.8	50.8	-12.1	38.7	44.8	-9.0	-0.1
60.3	49.7	33.0	2.8	7.2	8.7	17.3	8.0	2.4	3.5	3.3	-7.9	-0.7	-2.0	-2.0	
2-octanone 3															
-1.2	-2.1	-2.4	-1.4	5.6	3.6	-19.8	2.1	-13.9	-13.0	-5.6	6.4	11.8	34.5	52.1	14.2
-12.8	-0.3	4.6	-4.1	-5.6	8.0	-2.6	-8.0	5.3	1.2	1.6	2.1	5.4	12.5	19.7	-1.6
-8.9	-0.6	8.2	-6.1	-5.8	-0.2	-8.3	-2.6	-2.3	-1.9	1.9	7.1	-0.2	8.6	8.4	0.4
4.7	7.0	-14.9	12.5	14.4	12.7	3.3	51.4	13.9	24.5	58.1	-3.3	38.7	47.4	-1.7	0.2
57.1	51.1	41.1	6.6	16.2	22.0	22.2	20.6	16.4	9.1	14.3	9.2	0.3	7.2	6.2	
2-octanone 1															
3.7	5.2	5.6	16.5	22.7	21.6	4.6	19.5	8.0	6.6	10.9	31.6	7.0	23.0	45.3	9.0
4.6	12.1	16.4	12.3	11.0	23.5	6.6	2.0	10.9	9.2	11.4	11.1	2.4	9.9	19.5	0.2
0.6	7.7	8.3	-0.5	3.9	0.9	-9.5	-2.4	0.8	1.8	3.7	5.5	0.7	7.6	3.4	-0.8
-1.8	-0.7	-22.9	3.9	3.4	-0.7	5.0	44.5	0.6	22.0	53.4	-12.9	33.1	37.7	-11.6	-13.9
58.7	48.1	33.9	-1.6	2.0	5.2	8.2	8.6	1.5	5.1	3.1	-4.0	-4.6	-0.7	4.6	
Avg 2-octanone															
2.8	1.9	2.3	9.8	14.7	12.9	-2.3	7.4	-1.4	-4.0	-4.6	-0.7	4.6	-4.0	-8.0	14.7
-0.1	8.0	9.2	2.7	1.4	10.7	0.7	-4.6	3.8	3.2	5.2	4.4	2.5	8.6	17.2	-0.1
-2.3	2.4	6.6	0.4	5.0	2.5	0.5	8.8	7.9	-1.5	-0.3	2.9	-0.1	4.1	1.5	-1.2
8.9	12.3	-5.0	3.3	4.1	0.4	1.4	40.2	5.5	20.6	51.2	-10.3	40.1	47.0	-5.8	0.2
57.8	48.7	33.6	3.5	10.0	14.2	20.7	14.1	11.4	5.4	8.3	-1.0	0.7	0.1	0.2</td	

