SUPPORTING INFORMATION

Predicting the gas/particle distribution of SVOCs in the indoor environment using poly-parameter Linear Free Energy Relationships

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1 McGowan volume

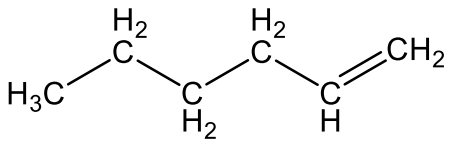
Table SI-1: Characteristic atomic volumes as described by Abraham and McGowan (1987).

Atom	Characteristic volume
C (cm³/mol)	16.35
H (cm³/mol)	8.71
O (cm³/mol)	12.43
N (cm³/mol)	14.39
F (cm³/mol)	10.48
Cl (cm³/mol)	20.95
Br (cm³/mol)	26.21
P (cm³/mol)	24.87
Si (cm³/mol)	26.83

Procedure:

Sum characteristic atomic volumes (cm³/mol) and substract 6.56 cm³/mol for each bond (double and triple bonds count 1).

Example 1-hexene:



V = (6 * 16.35) + (12 * 8.71) - (17 * 6.56) = 91.1

2 Aerosol descriptors

Table SI-2: Descriptors of outdoor aerosols as determined by Arp et al. (2008a, 2008b) for a temperature of T = 15 °C (288 K) and a relative humidity of RH = 50%.

Aerosol	s	a	b	v	l	c	T (K)
Aerosol Aspvreten	0.95	2.52	0.55	0.49	0.64	-5.95	288
Aerosol Berlin Spring	1.01	3.17	0.30	0.51	0.78	-7.42	288
Aerosol Berlin Winter	1.38	3.21	0.42	0.98	0.63	-7.24	288
Aerosol Duebendorf Fall	1.19	3.37	0.03	0.73	0.66	-7.08	288
Aerosol Duebendorf Spring	1.14	2.75	0.45	0.69	0.61	-6.48	288
Aerosol Duebendorf Summer	1.09	2.91	0.48	0.71	0.66	-7.28	288
Aerosol Duebendorf Winter	1.63	3.20	0.28	1.51	0.51	-7.33	288
Aerosol Roost	1.45	3.12	0.37	0.86	0.60	-6.99	288
Aerosol Zürich	1.09	2.99	0.64	0.35	0.75	-6.84	288

3 Properties of outdoor and indoor aerosols

Table SI-3: Comparison of outdoor and indoor aerosols: particle mass concentration, fraction of elemental carbon (f_{EC}) and fraction of organic carbon (f_{OC}).

Aerosol type	Location	$C_{Particle}$ (µg/m³)	f_{EC}	f_{OC}
Outdoor	Aerosol Aspvreten	8 [1)]	0.04	n.d.
Outdoor	Aerosol Berlin Spring	30 [1)]	n.d.	n.d.
Outdoor	Aerosol Berlin Winter	30 [1)]	0.14	0.22
Outdoor	Aerosol Duebendorf Fall	57 [1)]	0.09	0.22
Outdoor	Aerosol Duebendorf Spring	16 [1)]	n.d.	n.d.
Outdoor	Aerosol Duebendorf Summer	45 [1)]	n.d.	n.d.
Outdoor	Aerol Duebendorf Winter	22 [1)]	0.16	0.24

Outdoor	Aerosol Roost	n.d.	0.15	0.29
Outdoor	Aerosol Zuerich	142.2 [1)]	0.05	n.d.
Indoor	Apartment Winter (non smoker)	29.6 [2)]	0.14	0.34
Indoor	Apartment Spring (non smoker)	27.1 [2)]	0.10	0.48
Indoor	Nursery School Winter (non smoker)	52.6 [2)]	0.08	0.30
Outdoor	Multi use Building (14 day campaign)	12.58 [3)]	0.05	0.32
Indoor	Multi use Building (14 day campaign)	6.88 [3)]	0.05	0.41
Outdoor	School classrooms	24.2 [4)]	0.10	0.19
Indoor	School classrooms	118.2 [4)]	0.08	0.18
Outdoor	School classrooms	23 [5)]	0.06	0.20
Indoor	School classrooms	33 [5)]	0.04	0.29
Outdoor	Near roadside (mechanical ventilation)	78.4 [6)]	0.09	0.16
Indoor	Near roadside (mechanical ventilation)	55.4 [6)]	0.09	0.21
Outdoor	Near roadside (natural ventilation)	78.4 [6)]	0.09	0.19
Indoor	Near roadside (natural ventilation)	55.4 [6)]	0.09	0.23
Outdoor	Boston area homes	12.7 [7)]	0.07	0.25
Indoor	Boston area homes	19.4 [7)]	0.04	0.39

1) PM_{10} (Arp et al., 2008b)
2) Respirable particulate matter (RPM) (50-P of N = 27) (Fromme et al., 2005)
3) Aerosol mass concentration (50-P over a 4 day campaign) (Johnson et al., 2017)
4) PM_{10} (50-P over a 6 week campaign) (Fromme et al., 2008)
5) $PM_{2.5}$ (50-P of 39 schools) Rivas et al. (2014)
6) $PM_{2.5}$ (average concentrations) Ho et al. (2004)
7) PM_{10} (mean values of 12 h and 24 h sampling) Long et al. (2000)

4 Compounds

Table SI-4: Identifiers and properties of the investigated compounds. "log (K_{HdA})" is the logarithm of the hexadecane/air partitioning coefficient (also expressed as "L") for T = 298 K.

Compound	**DEP**
Full name	Diethyl phthalate
CAS	84-66-2
SMILES	O=C(OCC)C1=CC=CC=C1C(=O)OCC
Molecular formula	C12H14O4
Molecular weight (g/mol)	222.2
log (K_{OA}) from SPARC	8.32
log (K_{OA}) from pp-LFER	7.79 (wet octanol); 7.42 (dry octanol)
log (K_{HdA}) from SPARC	7.32

Compound	**DnBP**
Full name	Di-n-butyl phthalate
CAS	84-74-2
SMILES	O=C(OCCCC)C1=CC=CC=C1C(=O)OCCCC
Molecular formula	C16H22O4
Molecular weight (g/mol)	278.4
log (K_{OA}) from SPARC	9.83
log (K_{OA}) from pp-LFER	9.43 (wet octanol); 9.20 (dry octanol)
log (K_{HdA}) from SPARC	9.28

Compound	**DiBP**
Full name	Di-iso-butyl phthalate
CAS	84-69-5
SMILES	O=C(OCC(C)C)C1=CC=CC=C1C(=O)OCC(C)C
Molecular formula	C16H22O4

Molecular weight (g/mol)	278.4
log (K_{OA}) from SPARC	9.62
log (K_{OA}) from pp-LFER	9.25 (wet octanol); 9.02 (dry octanol)
log (K_{HdA}) from SPARC	8.99

Compound	**DPP**
Full name	Dipentyl phthalate
CAS	131-18-0
SMILES	O=C(OCCCCC)C1=CC=CC=C1C(=O)OCCCCC
Molecular formula	C18H26O4
Molecular weight (g/mol)	306.4
log (K_{OA}) from SPARC	10.72
log (K_{OA}) from pp-LFER	10.33 (wet octanol); 10.22 (dry octanol)
log (K_{HdA}) from SPARC	10.31

Compound	**BBzP**
Full name	Butylbenzyl phthalate
CAS	85-68-7
SMILES	O=C(OCC1=CC=CC=C1)C2=CC=CC=C2C(=O)OCCCC
Molecular formula	C19H20O4
Molecular weight (g/mol)	312.4
log (K_{OA}) from SPARC	11.59
log (K_{OA}) from pp-LFER	11.08 (wet octanol); 11.62 (dry octanol)
log (K_{HdA}) from SPARC	11.06

Compound	**DEHP**
Full name	Di-2-ethylhexyl phthalate
CAS	117-81-7

SMILES	O=C(OCC(CCCC)CC)c(c(ccc1)C(=O)OCC(CCCC)CC)c1
Molecular formula	C24H38O4
Molecular weight (g/mol)	390.6
log (K_{OA}) from SPARC	12.89
log (K_{OA}) from pp-LFER	13.02 (wet octanol); 13.12 (dry octanol)
log (K_{HdA}) from SPARC	12.93

Compound	**DnBA**
Full name	Di-n-butyl adipate
CAS	105-99-7
SMILES	O=C(OCCCC)CCCCC(=O)OCCCC
Molecular formula	C14H26O4
Molecular weight (g/mol)	258.4
log (K_{OA}) from SPARC	8.14
log (K_{OA}) from pp-LFER	9.01 (wet octanol); 8.89 (dry octanol)
Log (K_{HdA}) from SPARC	7.67

Compound	**DIBA**
Full name	Di-iso-butyl adipate
CAS	141-04-8
SMILES	O=C(OCC(C)C)CCCCC(=O)OCC(C)C
Molecular formula	C14H26O4
Molecular weight (g/mol)	258.4
log (K_{OA}) from SPARC	7.93
log (K_{OA}) from pp-LFER	8.70 (wet octanol); 8.63 (dry octanol)
log (K_{HdA}) from SPARC	7.40

Compound	**DEHA**

Full name	Di-2-ethylhexyl adipate
CAS	103-23-1
SMILES	O=C(OCC(CC)CCCC)CCCCC(=O)OCC(CC)CCCC
Molecular formula	C22H42O4
Molecular weight (g/mol)	370.6
log (K_{OA}) from SPARC	11.29
log (K_{OA}) from pp-LFER	12.21 (wet octanol); 12.51 (dry octanol)
log (K_{HdA}) from SPARC	11.38

Compound	**DEHTP**
Full name	Di-2-ethylhexyl terephthalate
CAS	6422-86-2
SMILES	O=C(OCC(CC)CCCC)C1=CC=C(C=C1)C(=O)OCC(CC)CCCC
Molecular formula	C24H38O4
Molecular weight (g/mol)	390.6
log (K_{OA}) from SPARC	12.52
log (K_{OA}) from pp-LFER	13.07 (wet octanol); 13.45 (dry octanol)
log (K_{HdA}) from SPARC	12.71

Compound	**TOTM**
Full name	Tri-2-ethylhexyltrimellitate
CAS	3319-31-1
SMILES	O=C(OCC(CC)CCCC)C=1C=CC(C(=O)OCC(CC)CCCC)=C(C1)C(=O)OCC(CC)CCCC
Molecular formula	C33H54O6
Molecular weight (g/mol)	546.8
log (K_{OA}) from SPARC	17.89
log (K_{OA}) from pp-LFER	18.16 (wet octanol); 18.78 (dry octanol)

log (K_{HdA}) from SPARC	17.89

Compound	**TEHP** (solid at room temperature)
Full name	Tri-2-ethylhexyl phosphate
CAS	78-42-2
SMILES	O=P(OCC(CC)CCCC)(OCC(CC)CCCC)OCC(CC)CCCC
Molecular formula	C24H51O4P
Molecular weight (g/mol)	434.6
log (K_{OA}) from SPARC	12.01
log (K_{OA}) from pp-LFER	13.07 (wet octanol); 13.68 (dry octanol)
log (K_{HdA}) from SPARC	12.94

Compound	**TPP** (solid at room temperature)
Full name	Triphenyl phosphate
CAS	115-86-6
SMILES	O=P(OC1=CC=CC=C1)(OC2=CC=CC=C2)OC3=CC=CC=C3
Molecular formula	C18H15O4P
Molecular weight (g/mol)	326.3
log (K_{OA}) from SPARC	10.33
log (K_{OA}) from pp-LFER	11.11 (wet octanol); 10.48 (dry octanol)
log (K_{HdA}) from SPARC	10.84

Compound	**DINCH** (mixture of isomers)
Full name	1,2-Cyclohexane dicarboxylic acid diisononyl ester
CAS	166412-78-8 Hexamoll® DINCH (Europe and Asia) 474919-59-0 Hexamoll® DINCH (United States)
SMILES [1)]	O=C(OCCCCCCC(C)C)C1C(C(=O)OCCCCCCC(C)C)CCCC1
Molecular formula	C26H48O4

Molecular weight (g/mol)	424.7
log (K_{OA}) from SPARC	12.88 (calculated for the selected isomer)
log (K_{OA}) from pp-LFER	14.09 (wet octanol); 14.53 (dry octanol)
log (K_{HdA}) from SPARC	13.12 (calculated for the selected isomer)

1) SMILES is for the isomer bis(7-methyloctyl) 1,2-cyclohexanedicarboxylate

Calculation of the octanol/air distribution coefficient K_{OA} from SPARC requires the octanol/water distribution coefficient K_{OW} and Henry's constant H (mol/(l·atm)). Then, K_{OA} can be obtained from equations (SI-1) and (SI-2).

$$K_{OA} = K_{OW} \cdot R \cdot T \cdot H \quad \text{(SI-1)}$$

$$\log (K_{OA}) = \log (K_{OW}) + \log (H) + 1.389 \quad \text{(SI-2)}$$

R = 0.0821 l·atm/(K·mol); T = 298 K.

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