Table S1. Caption. Experimental (exp.) and calculated (calc.) densities of the 310 fluids
in the training set used to parametrize the present vdW model.

Fluids without hydrogen bonds:	exp.	calc.
Isopentane	0.6201	0.6640
Pentane	0.6262	0.6610
Hexane	0.6548	0.6810
2-Methyl-2-butene	0.6630	0.6980
trans-3-Hexene	0.6780	0.6980
Heptane	0.6837	0.6940
Hydrogen cyanide	0.6840	0.7350
2,2,3-Trimethylbutane	0.6901	0.7210
Dimethylacetylene	0.6910	0.6960
2,3-Dimethylhexane	0.6912	0.7240
2,2-Dimethylhexane	0.6953	0.7110
2,4-Dimethylhexane	0.6962	0.7190
2-Methylheptane	0.6980	0.7070
Octane	0.6986	0.6840
1,1,2,2-Tetramethylcyclopropane	0.7020	0.7530
4-Methylheptane	0.7046	0.7150
5,5-Dimethylhexene	0.7050	0.7350
3-Methylheptene	0.7070	0.7260
2-Methylheptene	0.7104	0.7230
Diethylether	0.7138	0.7470
Nonane	0.7176	0.7130
2,3,4-Trimethylpentane	0.7191	0.7390
3-Ethyl-2-methylpentane	0.7193	0.7240
3-Methylhept-3-ene	0.7240	0.7310
2,2,3-Trimethylpentane	0.7262	0.7410
3-Ethyl-3-methylpentane	0.7274	0.7350
2-Methylnonane	0.7281	0.7230

Decane	0.7300
	0.7110
4-Methylnonane	0.7323
	0.7300
5-Methylnonane	0.7326
	0.7300
3-Methylnonane	0.7354
	0.7240
Undecane	0.7402
	0.7270
cis-1,3-Dimethylcyclopentane	0.7402
	0.7660
Methylcyclopentane	0.7440
	0.7640
trans-1,3-Dimethylcyclopentane	0.7443
	0.7660
Cyclopentane	0.7457
	0.7500
trans-1,2-Dimethylcyclopentane	0.7468
	0.7710
Dodecane	0.7487
	0.7240
1,1-Dimethylcyclopentane	0.7499
	0.7750
Tridecane	0.7564
	0.7370
Tetradecane	0.7628
	0.7280
Cycloheptane	0.7655
	0.7920
Cyclohexane	0.7658
	0.7750
Triisobutylamine	0.7680
	0.7740
cis-1,2-Dimethylcyclopentane	0.7680
	0.7680
Pentadecane	0.7685
	0.7440
1,2-Bimethylene-cyclobutane	0.7698
	0.8010
Cyclooctane	0.7728
	0.8170
Divinyl ether	0.7730
	0.8370
Hexadecane	0.7733
	0.7330
Cyclononane	0.7788
	0.8040
Propionitrile	0.7820
	0.7680
Acetaldehyde	0.7834
	0.8100
Cyclodecane	0.7842
	0.8320
Acetonitrile	0.7857
	0.7620
1,6-Heptadien-3-yne	0.7870
	0.7870
Acetone	0.7899
	0.8060
Cyclopentadiene	0.7928
	0.8370
Pentan-2-one	0.8060

	0.7980	
Acrylnitrile		0.8060
	0.8340	
1,5-Heptadiyne		0.8100
	0.7830	
2,4,6-Trimethyl-3,5-dioxyheptane		0.8120
	0.8350	
Crotonitrile		0.8240
	0.8160	
Acrolein		0.8390
	0.8710	
1-Nonanethiol		0.8420
	0.8170	
Dimethylsulfide		0.8480
	0.8620	
Carene		0.8560
	0.8450	
p-Xylene		0.8611
	0.8660	
Cumene		0.8618
	0.8640	
m-Xylene		0.8642
	0.8770	
Mesitylene		0.8650
	0.8580	
Toluene		0.8669
	0.8720	
tert-Butylbenzene		0.8670
	0.8510	
Ethylbenzene		0.8670
	0.8660	
trans-Decalin		0.8700
	0.8560	
Benzene		0.8765
	0.8910	
o-Xylene		0.8802
	0.8800	
Tetrahydrofuran		0.8892
	0.8750	
1-Chloropropane		0.8910
	0.8900	
Cyclopropanenitrile		0.8950
	0.8560	
Methylthioethene		0.9026
	0.8980	
Styrene		0.9060
	0.9090	
Norbonadiene		0.9090
	0.9360	
Methylpropionate		0.9150
	0.9280	
Nonanedioic acid, di-2-ethylhexyl ester		0.9150
	0.8970	
Ethylformate		0.9168
	0.9410	
1,3,5,7-Cyclooctatetraene		0.9206
	0.9400	
2,6-Dimethylpyridine		0.9230
	0.9230	
2-Propene-1-thiol		0.9250
	0.9030	
Vinylacetate		0.9320
	0.9710	

1,2-Epithiopropane	0.9410
	0.9580
2-Methylpyridine	0.9440
	0.9380
Cyclohexanone	0.9478
	0.9240
Cyclopentanone	0.9487
	0.9230
Furan	0.9514
	0.9960
3-Methylpyridine	0.9520
	0.9360
4-Methylpyridine	0.9550
	0.9430
N,N'-Dimethylaniline	0.9557
	0.9280
Dipropyl disulfide	0.9599
	0.9920
1,2-bis-2,2'-dimethyldiaziridinyl ethane	0.9600
	0.9100
Indan	0.9639
	0.9570
Butyne dinitrile	0.9700
	1.0620
1,2,1',2'-tetramethyl-3,3'-bidiaziridinyl	0.9700
	0.9190
Tetramethylurea	0.9710
	0.9110
2,4-Pentanedione	0.9721
	0.9590
Diethyl Azelate	0.9729
	0.9520
Methylformate	0.9742
	0.9890
Cumenaldehyde	0.9755
	0.9630
Azidocyclohexane	0.9790
	0.9620
2,3-Butanedione	0.9808
	0.9770
Pyridine	0.9819
	0.9690
Azidocyclopentane	0.9850
	0.9620
Thiocyclohexane	0.9861
	0.9650
Pentanedinitrile	0.9910
	0.9120
Paraldehyde	0.9940
	1.0210
Anisole	0.9940
	0.9810
Indene	0.9960
	1.0060
Tetrahydrothiophene	0.9987
	0.9750
2-Methylnaphthalene	1.0058
	1.0020
Nicotine	1.0100
	0.9940
Benzonitrile	1.0100
	1.0110
2-Methylthiophene	1.0190

	1.0480	
Thiacyclobutane		1.0200
	0.9790	
1-Methylnaphthalene		1.0202
	1.0120	
3-Methylthiophene		1.0220
	1.0510	
N-Methyl-2-pyrrolidone		1.0230
	0.9630	
3-Butyl-4-propylfuroxan		1.0260
	0.9850	
3-Hexyl-4-methylfuroxan		1.0270
	0.9820	
3-Chloro-1-propyne		1.0300
	1.0140	
p-Dioxane		1.0340
	1.0030	
2-Methylbenzenethiol		1.0410
	1.0410	
Benzaldehyde		1.0415
	1.0460	
Dimethylfurazan		1.0530
	1.0470	
4-azidotoluene		1.0530
	1.0600	
Thioanisole		1.0579
	1.0390	
Benzenemethanethiol		1.0580
	1.0390	
2-Methyl-quinoline		1.0600
	1.0680	
1,3-Dioxolane		1.0600
	1.0180	
1,5-Diazidobutane		1.0600
	1.0050	
Dimethyldisulfide		1.0630
	1.0680	
Thiophene		1.0649
	1.1100	
2-Azidotoluene		1.0650
	1.0720	
Azidomethylbenzene		1.0660
	1.0590	
Diphenylether		1.0661
	1.0730	
Thiophenol		1.0775
	1.0830	
Isoxazole		1.0780
	1.0950	
Pyrimidine		1.0790
	1.0420	
1,4-Diazidobutane		1.0790
	1.0320	
Oxazole		1.0800
	1.0960	
Acetic anhydride		1.0820
	1.1160	
Azidobenzene		1.0860
	1.0920	
Methylbenzoate		1.0933
	1.0900	
Quinoline		1.0977
	1.0890	

Chloromethylbenzene	1.1000
	1.0770
Dimethylsulfoxyde	1.1014
	1.0080
Pyridazine	1.1035
	1.0450
Acetyl chloride	1.1040
	1.1530
Chlorobenzene	1.1058
	1.1230
Diphenyl sulfide	1.1136
	1.1210
3-Azidomethyl-3-ethyloxetane	1.1200
	1.0160
Carbonyl cyanide	1.1240
	1.2110
Butyrolactone	1.1280
	1.0720
Nitromethane	1.1371
	1.1170
6-Methyl-3-nitroso-1,3,5-triazabicyclo[3.1.0]hexane	1.1400
	1.1650
2-Oxetanone	1.1460
	1.0900
m-Nitrotoluene	1.1570
	1.1620
m-Difluorobenzene	1.1570
	1.1370
Furfural	1.1590
	1.1470
o-Difluorobenzene	1.1600
	1.1440
o-Nitrotoluene	1.1630
	1.1570
p-Difluorobenzene	1.1700
	1.1380
1,2-bis-2-Azidoethyl diaziridine	1.1700
	1.0710
1,1-Dichloroethane	1.1757
	1.1930
1-Chloro-2,3-epoxypropane	1.1810
	1.1060
Trifluoromethylbenzene	1.1880
	1.1780
2-Chloroanisole	1.2020
	1.1530
4-Methyl-1,2-doxalan-2-one	1.2060
	1.1700
2,2,2-Trichlorotrimethylamine	1.2090
	1.1700
Benzoyl chloride	1.2120
	1.2440
1,1-Dichloroethylene	1.2130
	1.2780
1-Bromopentane	1.2180
	1.1940
1,2-Dichloroethane	1.2351
	1.1900
3-Methyl-2,5-furandione	1.2470
	1.2800
bis-1,3-Diazidoisopropyladipate	1.2540
	1.3100
2-Nitroanisole	1.2540

	1.2240	
Carbon disulfide		1.2555
	1.4410	
1,2,4-Triazidobutane		1.2660
	1.1640	
Bis (2-chloroethyl) sulphide		1.2740
	1.1880	
cis-1,2-Dichloroethylene		1.2840
	1.2890	
m-Dichlorobenzene		1.2884
	1.2980	
o-Dichlorobenzene		1.3059
	1.3180	
Dichloromethane		1.3266
	1.3010	
Dichlodimethylether		1.3280
	1.2810	
Dihydrogen disulfide		1.3340
	1.2690	
1-Bromopropane		1.3540
	1.3490	
3,4-bis(azidomethyl)furazan		1.3620
	1.3450	
Methylnitroglycol		1.3770
	1.4330	
1,1,1-Trifluoro-2-nitroethane		1.3910
	1.4160	
1-Fluoro-1,1-dinitroethane		1.4000
	1.4990	
1,1,1-Trifluoro-3-nitropropane		1.4200
	1.3160	
Bromomethylbenzene		1.4380
	1.4040	
1,1,2-Trichloroethane		1.4397
	1.3950	
((2-Fluoro-2,2-dinitro-ethoxy)methyl) oxirane		1.4500
	1.4300	
Dinitrogen tetroxide		1.4500
	1.7040	
1,2,4-Trichlorobenzene		1.4590
	1.4510	
Trichloroethylene		1.4620
	1.4980	
Trithiocarbonic acid		1.4700
	1.4700	
Trichloromethane		1.4832
	1.5280	
Perfluoroacetic anhydride		1.4900
	1.6240	
1,1,7-Trihydroperfluoroheptyl acrylate		1.5000
	1.5470	
Perfluorothiophenol		1.5010
	1.5240	
1,1',1'',2-Tetrachloroethane		1.5406
	1.5430	
Perfluorobenzonitrile		1.5630
	1.4440	
3-Bromo-1-propyne		1.5790
	1.5380	
Tetrachloromethane		1.5940
	1.7000	
1,1',2,2'-Tetrachloroethane		1.5953
	1.5600	

Perfluorobenzene	1.6180	1.4710
Tetrachloroethylene	1.6200	1.6510
1,1,1,4,4,7-Hexafluoro-7,7-dinitro-3,5-dioxaheptane	1.6200	1.6460
1-Bromo-3-chlorobenzene	1.6300	1.6460
1-Bromo-2-chlorobenzene	1.6390	1.6620
Nitrogen trichloride	1.6530	1.5910
Nitrotrichloromethane	1.6570	1.7770
Chloroformic acid	1.6600	1.7790
Acetyl bromide	1.6630	1.7320
Perfluorobutanoic anhydride	1.6650	1.7300
1,1,1,7,7,13,13,13-Octafluoro-4,4,10,10-tetranitro-2,6,8,12-tetraoxatridecane	1.6650	1.6920
Pentachloroethane	1.6796	1.6630
1,1,4,4,7-Pentafluoro-1,7,7-trinitro-3,5-dioxoheptane	1.6800	1.6770
1-Trifluoromethyl-3,5-dinitrobenzene	1.6900	1.5660
Perfluorohexane	1.6995	1.7000
Perfluoroheptane	1.7333	1.7350
2,2,3-Trichloro-1,1,1,3,4,4,4-heptafluorobutane	1.7484	1.7690
Perfluoromethyl cyclohexane	1.7878	1.8120
1,2-Dimethylperfluorocyclohexane	1.8290	1.8840
2,2,3-Tribromobutane	2.1723	2.1270

Fluids with hydrogen bonds:	exp.	calc.
2-Aminopropame	0.6890	0.7360
Dimethylamine	0.7056	0.7320
1-Aminopropane	0.7170	0.7310
2-Aminobutane	0.7250	0.7430
2-Pentanamine	0.7384	0.7590
1-Aminobutane	0.7410	0.7410
3-Pentanamine	0.7487	0.7590
1-Pentanamine	0.7544	0.7400
Hexylamine	0.7660	

	0.7560	
Heptanamine		0.7754
	0.7580	
Octanamine		0.7826
	0.7670	
Isopropanol		0.7855
	0.7950	
1,1-Dimethylhydrazine		0.7860
	0.7980	
Nonamine		0.7886
	0.7630	
Ethanol		0.7890
	0.7900	
Methanol		0.7914
	0.7860	
Decanamine		0.7936
	0.7670	
Undecanamine		0.7979
	0.7680	
Butan-2-ol		0.8030
	0.8070	
Propanol		0.8035
	0.7930	
Pentan-2-ol		0.8100
	0.8100	
Butan-1-ol		0.8100
	0.7940	
Pentanol		0.8140
	0.7970	
Hexanol		0.8190
	0.8010	
Cyclohexanamine		0.8191
	0.8710	
Pentan-3-ol		0.8210
	0.8060	
Heptanol		0.8220
	0.7930	
Octanol		0.8260
	0.7960	
1,2-Dimethylhydrazine		0.8270
	0.7970	
Nonanol		0.8273
	0.7920	
Undecanol		0.8298
	0.7890	
Decanol		0.8300
	0.7990	
Aziridine		0.8330
	0.7900	
allyl alcohol		0.8550
	0.8550	
Pyrrolidine		0.8586
	0.8440	
Monomethylhydrazine		0.8740
	0.8370	
1,3-Propanediamine		0.8840
	0.8500	
Polargonic acid		0.9052
	0.8930	
Caprylic acid		0.9106
	0.8950	
Enanthylic acid		0.9181
	0.9210	

Caproic acid	0.9274	0.9530
Valeric acid	0.9390	0.9740
Butyric acid	0.9580	1.0010
Pyrrole	0.9698	0.9520
2,4-Xylidine	0.9720	0.9630
N,N-di(2-propinyl) hydrazine	0.9760	0.9400
2,6-Xylidine	0.9840	0.9760
m-Toludine	0.9890	0.9710
N-Methylaniline	0.9891	0.9500
Propionic acid	0.9930	1.0580
o-Toludine	0.9980	0.9850
Water	0.9982	0.9220
2,3-Butanediol	1.0000	0.9780
Hydrazine	1.0036	0.9080
2-Propinyl hydrazine	1.0090	0.9210
Methacrylic acid	1.0150	1.0820
Aniline	1.0217	1.0030
m-Cresol	1.0341	1.0240
Benzene methanol	1.0419	1.0280
Acetic acid	1.0492	1.1430
Acrylic acid	1.0510	1.1640
Cyclopropane carboxylic acid	1.0890	1.1160
Glycidol	1.1140	1.0730
2-Furanmethanol	1.1296	1.2720
2-azidoethanol	1.1490	1.1760
Formic acid	1.2200	1.3020
1,3-Diazidopropan-2-ol	1.2600	1.2930
o-Chlorophenol	1.2634	1.3170
1,3-Diazido-2-nitrazopropane	1.4320	1.4700
Hydrogen peroxide	1.4400	1.3870
2-acryloylamino-1,2,4,5-tetradeoxy-1,4,5-tris(difluoroamino)pentitol	1.4690	1.4200
Perfluoroacetic acid	1.5351	

1.5680		
Nitric acid		1.5856
1.8890		
Perfluorobutanoic acid		1.6510
1.6890		

Table S2. Densities of the 36 liquids of the test set
(not included in the training set of Table S1).

		exp.	ACD	vdW
1	N-Ethyl N-methyl ethanamine	0.703	0.736	0.726
2	4-Methylcyclopentene	0.763	0.805	0.788
3	4-Undecyne	0.775	0.787	0.749
4	2-Methyl-3-butyn-2-amine	0.790	0.843	0.824
5	1-Fluoroheptane	0.806	0.790	0.777
6	2,3-Dimethyl cis-oxirane	0.823	0.855	0.833
7	Tridecyl cyclohexane	0.824	0.857	0.790
8	1,1'-Methylene bisoxy bispropane	0.835	0.843	0.830
9	1-Hexyn-3-ol	0.870	0.898	0.867
10	Acetic acid 2-ethylhexylester	0.872	0.872	0.871
11	2-Chloro-1-propene	0.902	0.907	0.948
12	4-Tetradecenoic acid	0.902	0.913	0.877
13	2-Chloro-1,3-butadiene	0.956	0.922	0.987
14	3-Oxobutylester butanoic acid	0.967	0.981	0.969
15	2-Nitrobutane	0.968	0.957	0.965
16	Tetrahydro-2H-thiopyran	0.986	0.964	0.970
17	1,1-Dimethylether ester acid nitric	1.014	1.047	1.089
18	Acetyl fluoride	1.032	0.967	1.011
19	2,5-Dichlorohexane	1.047	1.026	1.019
20	Acetyl chloride	1.105	1.120	1.153
21	Carbonochloridic acid ethylester	1.135	1.167	1.180
22	Cyanic acid	1.140	1.197	1.239
23	4-Methyl-1,3-dioxolan-2-one	1.205	1.169	1.176
24	Trinitromethane	1.479	1.803	1.793
25	Chlorosulfuric acid methylester	1.480	1.557	1.564
26	Butanoic acid heptafluoromethylester	1.483	1.492	1.492
27	Terrazole	1.503	1.574	1.522
28	Trichlorofluoroethene	1.546	1.582	1.592
29	Tetranitromethane	1.638	2.037	2.048
30	Trinitrochloromethane	1.677	1.956	1.950
31	2,3-Dichloro-1,1,1,2,3,4,4,4-octafluorobutane	1.680	1.681	1.707
32	1,2-dichloro-3,3,4,4,5,5,6,6-octafluorocyclohexane	1.719	1.740	1.710
33	Bromochlorodinitromethane	2.039	2.304	2.252
34	Dibromodinitromethane	2.444	2.719	2.617
35	Dibromochloromethane	2.451	2.408	2.557
36	Tribromonitromethane	2.811	3.056	2.909

Table S3. Densities of the 11 isomers with formula C8H11N: experimental values (exp) ; values calculated using the present van der Waals scheme (vdW) ; the ACD group contribution method (ACD) or the Piacenza approach assuming a reduced intermolecular volume of 0.7362.

	exp.	vdW	ACD	ve=0.7362
2-Propyl pyridine	0.912	0.900	0.918	0.898
3,1-Methylethyl pyridine	0.922	0.908	0.912	0.901
2,1-Methylethyl pyridine	0.934	0.905	0.912	0.897
4,1-Methylethyl pyridine	0.938	0.930	0.912	0.901
4-Methyl-benzene-methanamine	0.952	0.944	0.964	0.899
N-Ethyl aniline	0.963	0.934	0.966	0.903
p-Ethyl aniline	0.968	0.952	0.973	0.908
3,5-Xylidine	0.971	0.954	0.975	0.908
2-Methyl benzene methanamine	0.977	0.958	0.964	0.898
2,5-Xylidine	0.979	0.957	0.975	0.905
2-Ethyl aniline	0.983	0.967	0.973	0.904