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A Linear Solvation Energy Relationship to Predict Vapor Pressure from Molecular Structure

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Table S1. Parameters and log P_{vap} values used to develop the LSER

No.	Compound	P_{vap} (Pa)	Source	Error	log P_{vap}	Predicted log P_{vap}	A	B	V	E	S	λ	η
1	n-pentane	6.84E+04	E	<3%	4.835	4.984	0	0	0.813	0	0	0	0
2	isopentane	9.17E+04	EP	<3%	4.962	4.984	0	0	0.813	0	0	0	0
3	n-hexane	2.03E+04	E	<3%	4.307	4.484	0	0	0.954	0	0	0	0
4	3-methylpentane	2.52E+04	E	<3%	4.402	4.484	0	0	0.954	0	0	0	0
5	n-heptane	6.07E+03	E	<3%	3.783	3.984	0	0	1.095	0	0	0	0
6	n-octane	1.87E+03	E	<3%	3.272	3.485	0	0	1.236	0	0	0	0
7	n-nonane	5.80E+02	E	<3%	2.764	2.986	0	0	1.377	0	0	0	0
8	n-decane	1.81E+02	E	<3%	2.258	2.486	0	0	1.518	0	0	0	0
9	n-undecane	5.56E+01	E	<3%	1.745	1.985	0	0	1.659	0	0	0	0
10	n-dodecane	1.79E+01	E	<3%	1.252	1.489	0	0	1.799	0	0	0	0
11	n-tridecane	5.69E+00	E	<1%	0.755	0.988	0	0	1.940	0	0	0	0
12	n-tetradecane	1.86E+00	E	<3%	0.270	0.489	0	0	2.081	0	0	0	0
13	n-pentadecane	6.55E-01	E	<3%	-0.184	-0.011	0	0	2.222	0	0	0	0
14	n-hexadecane	1.99E-01	E	<3%	-0.700	-0.510	0	0	2.363	0	0	0	0
15	n-heptadecane	6.62E-02	E	<5%	-1.179	-1.009	0	0	2.504	0	0	0	0
16	4-methylnonane	3.09E+02	EP	<3%	2.490	2.486	0	0	1.518	0	0	0	0
17	2-methyloctane	8.44E+02	E	<3%	2.927	2.986	0	0	1.377	0	0	0	0
18	3-methyloctane	8.33E+02	EP	<3%	2.921	2.986	0	0	1.377	0	0	0	0
19	2-methylpentane	2.81E+04	E	<3%	4.449	4.484	0	0	0.954	0	0	0	0
20	2-methylhexane	8.77E+03	E	<3%	3.943	3.984	0	0	1.095	0	0	0	0
21	3-methylhexane	8.19E+03	E	<3%	3.913	3.984	0	0	1.095	0	0	0	0
22	2-methylheptane	2.75E+03	E	<3%	3.439	3.485	0	0	1.236	0	0	0	0
23	3-methylheptane	2.61E+03	E	<3%	3.417	3.485	0	0	1.236	0	0	0	0
24	4-methylheptane	2.73E+03	E	<3%	3.436	3.485	0	0	1.236	0	0	0	0
25	3-ethylhexane	2.68E+03	E	<3%	3.428	3.485	0	0	1.236	0	0	0	0
26	3-methylnonane	2.64E+02	EP	<3%	2.421	2.486	0	0	1.518	0	0	0	0
27	2-methylnonane	2.51E+02	EP	<3%	2.400	2.486	0	0	1.518	0	0	0	0
28	5-methylnonane	2.94E+02	EP	<3%	2.468	2.486	0	0	1.518	0	0	0	0
29	4-methyloctane	9.10E+02	EP	<3%	2.959	2.986	0	0	1.377	0	0	0	0
30	3-methylundecane	2.57E+01	EP	<10%	1.411	1.489	0	0	1.799	0	0	0	0
31	neopentane	1.71E+05	E	<1%	5.234	4.984	0	0	0.813	0	0	0	0
32	2,2-dimethylbutane	4.27E+04	E	<3%	4.631	4.484	0	0	0.954	0	0	0	0
33	2,3-dimethylbutane	3.13E+04	E	<3%	4.496	4.484	0	0	0.954	0	0	0	0
34	2,2-dimethylpentane	1.40E+04	E	<3%	4.147	3.984	0	0	1.095	0	0	0	0
35	2,3-dimethylpentane	9.17E+03	E	<3%	3.962	3.984	0	0	1.095	0	0	0	0
36	2,4-dimethylpentane	1.31E+04	E	<3%	4.118	3.984	0	0	1.095	0	0	0	0
37	3,3-dimethylpentane	1.10E+04	E	<3%	4.042	3.984	0	0	1.095	0	0	0	0
38	2,2-dimethylhexane	4.54E+03	E	<3%	3.657	3.485	0	0	1.236	0	0	0	0
39	2,3-dimethylhexane	3.13E+03	E	<3%	3.495	3.485	0	0	1.236	0	0	0	0
40	2,4-dimethylhexane	4.05E+03	E	<1%	3.607	3.485	0	0	1.236	0	0	0	0
41	2,5-dimethylhexane	4.04E+03	E	<3%	3.606	3.485	0	0	1.236	0	0	0	0
42	3,3-dimethylhexane	3.81E+03	E	<3%	3.581	3.485	0	0	1.236	0	0	0	0

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Table S1. (cont.)

No.	Compound	P_{vap} (Pa)	Source	Error	Predicted log P_{vap}	log P_{vap}	*A*	*B*	*V*	*E*	*S*	λ	η
43	3,4-dimethylhexane	2.89E+03	E	<1%	3.461	3.485	0	0	1.236	0	0	0	0
44	2,2-dimethyloctane	4.85E+02	E	<3%	2.686	2.486	0	0	1.518	0	0	0	0
45	2,2-dimethylheptane	1.53E+03	EP	<5%	3.183	2.986	0	0	1.377	0	0	0	0
46	2,4,4-trimethylhexane	1.79E+03	EP	<5%	3.253	2.986	0	0	1.377	0	0	0	0
47	3-ethylpentane	7.75E+03	E	<3%	3.890	3.984	0	0	1.095	0	0	0	0
48	2,2,3-trimethylbutane	1.37E+04	E	<3%	4.135	3.984	0	0	1.095	0	0	0	0
49	2-methyl-3-ethylpentane	3.19E+03	E	<3%	3.503	3.485	0	0	1.236	0	0	0	0
50	3-methyl-3-ethylpentane	3.06E+03	E	<3%	3.486	3.485	0	0	1.236	0	0	0	0
51	2,2,3-trimethypentane	4.28E+03	E	<1%	3.631	3.485	0	0	1.236	0	0	0	0
52	2,2,4-trimethylpentane	6.58E+03	E	<3%	3.818	3.485	0	0	1.236	0	0	0	0
53	2,3,3-trimethylpentane	3.60E+03	E	<3%	3.556	3.485	0	0	1.236	0	0	0	0
54	2,3,4-trimethylpentane	3.62E+03	E	<3%	3.558	3.485	0	0	1.236	0	0	0	0
55	2,2,5-trimethylhexane	2.22E+03	E	<3%	3.347	2.986	0	0	1.377	0	0	0	0
56	3,3,5-trimethylheptane	5.57E+02	EP	<3%	2.746	2.486	0	0	1.518	0	0	0	0
57	3,3-diethylpentane	9.72E+02	EP	<3%	2.988	2.986	0	0	1.377	0	0	0	0
58	2,2,3,3-tetramethylpentane	1.27E+03	E	<3%	3.103	2.986	0	0	1.377	0	0	0	0
59	2,2,3,4-tetramethylpentane	1.69E+03	EP	<5%	3.228	2.986	0	0	1.377	0	0	0	0
60	2,2,4,4-tetramethylpentane	2.67E+03	E	<3%	3.427	2.986	0	0	1.377	0	0	0	0
61	2,3,3,4-tetramethylpentane	1.18E+03	E	<5%	3.073	2.986	0	0	1.377	0	0	0	0
62	2,2,3,3-tetramethylhexane	1.81E+02	E	<3%	2.258	2.486	0	0	1.518	0	0	0	0
63	2,2,5,5-tetramethylhexane	5.37E+02	EP	<3%	2.730	2.486	0	0	1.518	0	0	0	0
64	3-ethylheptane	9.03E+02	P	<5%	2.956	2.986	0	0	1.377	0	0	0	0
65	cyclopentane	4.23E+04	E	<3%	4.627	4.908	0	0	0.705	0.263	0.100	0	0
66	cyclohexane	1.30E+04	E	<1%	4.115	4.363	0	0	0.845	0.305	0.100	0	0
67	cis-decalin	1.05E+02	E	<5%	2.019	2.242	0	0	1.300	0.544	0.250	0	0
68	trans-decalin	1.65E+02	E	<5%	2.218	2.362	0	0	1.300	0.467	0.230	0	0
69	cycloheptane	2.91E+03	E	<3%	3.464	3.809	0	0	0.986	0.35	0.100	0	0
70	cyclooctane	7.52E+02	E	<3%	2.876	3.237	0	0	1.127	0.413	0.100	0	0
71	methylcyclopentane	1.83E+04	E	<3%	4.263	4.456	0	0	0.845	0.225	0.100	0	0
72	methylcyclohexane	6.14E+03	E	<3%	3.788	3.934	0	0	0.986	0.244	0.100	0	0
73	cis-1,2-dimethylcyclohexane	1.93E+03	E	<3%	3.286	3.391	0	0	1.127	0.281	0.100	0	0
74	trans-1,2-dimethylcyclohexane	2.58E+03	E	<3%	3.412	3.496	0	0	1.127	0.191	0.100	0	0
75	1-pentene	8.51E+04	E	<3%	4.930	4.906	0	0.07	0.770	0.093	0.080	0	0
76	2-methly-1-butene	8.13E+04	EP	<3%	4.910	4.941	0	0.07	0.770	0.063	0.080	0	0
77	2-methyl-2-butene	6.25E+04	E	<3%	4.796	4.829	0	0.07	0.770	0.159	0.080	0	0
78	1-hexene	2.47E+04	E	<3%	4.392	4.424	0	0.07	0.911	0.078	0.080	0	0
79	2-methyl-1-pentene	2.61E+04	E	<3%	4.416	4.410	0	0.07	0.911	0.09	0.080	0	0
80	1-heptene	7.51E+03	E	<3%	3.876	3.908	0	0.07	1.052	0.092	0.080	0	0
81	1-octene	2.33E+03	E	<3%	3.367	3.405	0	0.07	1.193	0.094	0.080	0	0
82	1-nonene	7.20E+02	E	<3%	2.857	2.910	0	0.07	1.334	0.09	0.080	0	0
83	1-decene	2.27E+02	E	<3%	2.355	2.409	0	0.07	1.475	0.093	0.080	0	0
84	1-undecene	6.71E+01	E	<3%	1.827	1.911	0	0.07	1.616	0.091	0.080	0	0
85	1-dodecene	2.65E+01	E	<3%	1.423	1.414	0	0.07	1.756	0.089	0.080	0	0
86	cyclohexene	1.19E+04	E	<3%	4.076	4.258	0	0.1	0.802	0.395	0.200	0	0
87	indene	1.45E+02	E	<5%	2.161	2.025	0	0.2	0.988	1.001	0.770	0	0
88	cis-2-pentene	6.60E+04	E	<1%	4.820	4.850	0	0.07	0.770	0.141	0.080	0	0
89	3-methyl-1-butene	1.20E+05	E	<3%	5.080	4.941	0	0.07	0.770	0.063	0.080	0	0
90	cyclopentene	5.04E+04	E	<3%	4.703	4.826	0	0.1	0.662	0.335	0.200	0	0
91	cycloheptene	3.34E+03	E	<3%	3.524	3.705	0	0.1	0.943	0.414	0.220	0	0
92	1-methylcyclopentene	1.55E+04	EP	<10%	4.190	4.332	0	0.1	0.802	0.33	0.200	0	0
93	1,3-butadiene	2.81E+05	E	<1%	5.449	5.065	0	0.1	0.586	0.32	0.230	0	0
94	1,4-pentadiene	9.80E+04	EP	<3%	4.991	4.768	0	0.1	0.727	0.185	0.200	0	0
95	2-methyl-1,3-butadiene	7.34E+04	E	<3%	4.866	4.574	0	0.1	0.727	0.313	0.230	0	0
96	1,5-hexadiene	2.96E+04	EP	<5%	4.471	4.262	0	0.1	0.868	0.191	0.200	0	0
97	1,4-hexadiene	2.33E+04	E	<3%	4.367	4.203	0	0.1	0.868	0.241	0.200	0	0
98	2,3-dimethyl-1,3-butadiene	2.02E+04	E	<3%	4.305	4.028	0	0.14	0.868	0.352	0.230	0	0
99	1,3-cyclohexadiene	1.30E+04	E	<3%	4.113	4.118	0	0.14	0.759	0.515	0.300	0	0
100	1,4-cyclohexadiene	8.72E+03	EP	<10%	3.940	4.058	0	0.17	0.759	0.501	0.350	0	0
101	1,5-cyclooctadiene	6.59E+02	EP	<5%	2.819	2.925	0	0.2	1.041	0.603	0.360	0	0
102	carbon tetrachloride	1.52E+04	E	<1%	4.182	4.134	0	0	0.739	0.458	0.380	0	0
103	1,4-dichlorobutane	5.08E+02	EP	<10%	2.706	2.687	0	0.17	0.917	0.413	0.950	0	0
104	dichloromethane	5.84E+04	E	<3%	4.766	4.795	0.1	0.05	0.494	0.387	0.570	0	0

Table S1. (cont.)

No.	Compound	P_{vap} (Pa)	Source	Error	Predicted log P_{vap}	log P_{vap}	A	B	V	E	S	λ	η
105	chloroform	2.62E+04	E	<3%	4.418	4.437	0.15	0.02	0.617	0.425	0.490	0	0
106	1,1-dichloroethane	3.03E+04	E	<3%	4.481	4.493	0.1	0.1	0.635	0.322	0.490	0	0
107	1,2-dichloroethane	1.06E+04	E	<1%	4.027	4.155	0.1	0.11	0.635	0.416	0.640	0	0
108	1,1,2-trichloroethane	3.09E+03	EP	<3%	3.489	3.565	0.13	0.13	0.757	0.499	0.680	0	0
109	1,2-dichloropropane	6.89E+03	EP	<3%	3.838	3.769	0.1	0.11	0.776	0.371	0.600	0	0
110	1,1,1-trichloroethane	1.66E+04	E	<5%	4.221	4.128	0	0.09	0.757	0.369	0.410	0	0
111	1,1,1,2-tetrachloroethane	1.60E+03	E	<3%	3.205	3.155	0.1	0.08	0.880	0.542	0.630	0	0
112	1,1,2,2-tetrachloroethane	7.65E+02	E	<5%	2.884	2.896	0.16	0.12	0.880	0.595	0.760	0	0
113	isopropyl chloride	6.87E+04	EP	<5%	4.837	4.808	0	0.12	0.654	0.177	0.350	0	0
114	isosbutyl chloride	2.00E+04	E	<5%	4.301	4.261	0	0.12	0.795	0.191	0.370	0	0
115	2-chloro-2-methylpropane	4.09E+04	EP	<5%	4.612	4.501	0	0.12	0.795	0.142	0.250	0	0
116	trichloroethylene	9.83E+03	E	<3%	3.992	4.157	0.08	0.03	0.715	0.524	0.370	0	0
117	tetrachloroethylene	2.47E+03	E	<3%	3.393	3.484	0	0	0.837	0.639	0.440	0	0
118	allyl chloride	4.88E+04	EP	<5%	4.688	4.466	0	0.05	0.611	0.327	0.560	0	0
119	cis-1,2-dichloroethene	2.72E+04	E	<3%	4.435	4.329	0.11	0.05	0.592	0.436	0.610	0	0
120	trans-1,2-dichloroethene	4.45E+04	E	<5%	4.648	4.647	0.09	0.05	0.592	0.425	0.410	0	0
121	n-propyl chloride	4.59E+04	E	<3%	4.662	4.686	0	0.1	0.654	0.216	0.400	0	0
122	n-butyl chloride	1.35E+04	E	<3%	4.131	4.194	0	0.1	0.795	0.21	0.400	0	0
123	sec-butyl chloride	2.09E+04	E	<3%	4.321	4.294	0	0.12	0.795	0.189	0.350	0	0
124	1-chloropentane	4.36E+03	E	<3%	3.640	3.696	0	0.1	0.936	0.208	0.400	0	0
125	pentachloroethane	4.89E+02	E	<5%	2.690	2.554	0.17	0.06	1.002	0.648	0.660	0	0
126	1,1-dichloroethene	7.99E+04	E	<5%	4.903	4.827	0	0.05	0.592	0.362	0.340	0	0
127	ethyl iodide	1.80E+04	E	<3%	4.254	4.210	0	0.15	0.649	0.64	0.400	0	0
128	n-propyl iodide	5.74E+03	E	<3%	3.759	3.718	0	0.15	0.790	0.634	0.400	0	0
129	tribromomethane	7.34E+02	EP	<5%	2.866	2.948	0.15	0.06	0.775	0.974	0.680	0	0
130	1.3-dichloropropane	2.43E+03	EP	<5%	3.386	3.513	0	0.17	0.776	0.408	0.740	0	0
131	halothane	4.01E+04	E	<5%	4.603	4.541	0.15	0.05	0.741	0.102	0.380	0	0
132	methyl bromide	2.18E+05	E	<3%	5.339	5.239	0	0.1	0.425	0.399	0.430	0	0
133	bromoethane	6.30E+04	E	<3%	4.799	4.827	0	0.12	0.565	0.366	0.400	0	0
134	1-bromopropane	1.84E+04	E	<3%	4.266	4.327	0	0.12	0.706	0.366	0.400	0	0
135	2-bromopropane	2.89E+04	E	<3%	4.460	4.443	0	0.14	0.706	0.332	0.350	0	0
136	1-bromobutane	5.59E+03	E	<5%	3.748	3.835	0	0.12	0.847	0.36	0.400	0	0
137	1-bromoheptane	1.70E+02	E	<3%	2.229	2.355	0	0.12	1.270	0.343	0.400	0	0
138	methyl iodide	5.40E+04	E	<3%	4.732	4.622	0	0.13	0.508	0.676	0.430	0	0
139	dibromomethane	6.03E+03	EP	<3%	3.780	3.888	0.1	0.1	0.600	0.714	0.670	0	0
140	diiodomethane	1.60E+02	E	<5%	2.205	2.407	0.05	0.23	0.766	1.453	0.690	0	0
141	1-iodohexane	1.53E+02	EP	<10%	2.185	2.243	0	0.15	1.212	0.615	0.400	0	0
142	1-iodobutane	1.81E+03	E	<3%	3.258	3.227	0	0.15	0.930	0.628	0.400	0	0
143	benzyl chloride	1.74E+02	P	<3%	2.240	2.187	0	0.33	0.980	0.821	0.820	0	0
144	chlorobenzene	1.59E+03	EP	<5%	3.200	3.065	0	0.07	0.839	0.718	0.650	0	0
145	o-dichlorobenzene	1.81E+02	E	<3%	2.257	2.256	0	0.04	0.961	0.872	0.780	0	0
146	m-dichlorobenzene	2.86E+02	E	<3%	2.457	2.361	0	0.02	0.961	0.847	0.730	0	0
147	o-chlorotoluene	4.70E+02	EP	<3%	2.672	2.514	0	0.07	0.980	0.762	0.650	0	0
148	p-chlorotoluene	3.72E+02	EP	<5%	2.570	2.550	0	0.07	0.980	0.705	0.670	0	0
149	1,2,4-trichlorobenzene	5.74E+01	E	<3%	1.759	1.648	0	0	1.084	0.98	0.810	0	0
150	m-dibromobenzene	3.58E+01	EP	<10%	1.554	1.384	0	0.04	1.066	1.17	0.880	0	0
151	bromobenzene	5.68E+02	E	<3%	2.754	2.568	0	0.09	0.891	0.882	0.730	0	0
152	fluorobenzene	1.03E+04	E	<3%	4.012	3.840	0	0.1	0.734	0.477	0.570	0	0
153	benzotrifluoride	4.97E+03	E	<5%	3.696	3.647	0	0.1	0.910	0.225	0.480	0	0
154	iodobenzene	1.42E+02	E	<3%	2.151	1.777	0	0.12	0.975	1.188	0.820	0	0
155	methyl ethyl sulfide	2.13E+04	E	<3%	4.329	4.369	0	0.28	0.695	0.39	0.380	0	0
156	di-n-propyl sulfide	8.89E+02	E	<3%	2.949	2.907	0	0.32	1.118	0.358	0.380	0	0
157	diethyl sulfide	8.02E+03	E	<3%	3.904	3.889	0	0.32	0.836	0.373	0.380	0	0
158	dimethyl sulfide	6.46E+04	E	<3%	4.810	4.853	0	0.29	0.554	0.404	0.380	0	0
159	thiophene	1.05E+04	E	<3%	4.022	3.940	0	0.15	0.641	0.687	0.560	0	0
160	diethyl disulfide	5.67E+02	EP	<3%	2.754	2.813	0	0.28	0.999	0.67	0.480	0	0
161	dimethyl disulfide	3.83E+03	E	<3%	3.583	3.843	0	0.28	0.717	0.695	0.440	0	0
162	carbon disulfide	4.78E+04	E	<1%	4.680	4.785	0	0.07	0.491	0.877	0.210	0	0
163	2-methylthiophene	3.30E+03	E	<3%	3.519	3.439	0	0.16	0.782	0.688	0.560	0	0
164	paraldehyde	1.46E+03	EP	<5%	3.164	3.049	0	0.68	1.022	0.136	0.680	0	0
165	diethylether	7.17E+04	E	<3%	4.856	4.846	0	0.45	0.731	0.041	0.250	0	0
166	diisopropyl ether	1.98E+04	E	<3%	4.297	3.986	0	0.41	1.013	0	0.190	0	0

Table S1. (cont.)

No.	Compound	P_{vap} (Pa)	Source	Error	Predicted log P_{vap}	log P_{vap}	A	B	V	E	S	λ	η
167	di-n-butyl ether	8.37E+02	EP	< 5%	2.923	2.896	0	0.45	1.295	0	0.250	0	0
168	methyl n-propyl ether	6.10E+04	E	< 5%	4.785	4.824	0	0.45	0.731	0.06	0.250	0	0
169	di-n-propyl ether	8.30E+03	E	< 5%	3.919	3.801	0	0.45	1.013	0.08	0.250	0	0
170	anisole	4.83E+02	E	< 3%	2.684	2.652	0	0.29	0.916	0.708	0.750	0	0
171	1,4-dioxane	5.09E+03	E	< 1%	3.707	3.926	0	0.64	0.681	0.329	0.750	0	0
172	1,2-propylene oxide	7.13E+04	E	< 5%	4.853	5.009	0	0.45	0.481	0.243	0.570	0	0
173	furan	8.00E+04	E	< 3%	4.903	4.728	0	0.13	0.536	0.369	0.530	0	0
174	tetrahydrofuran	2.15E+04	E	< 1%	4.333	4.532	0	0.48	0.622	0.289	0.520	0	0
175	propanal	4.25E+04	E	< 3%	4.628	4.708	0	0.45	0.547	0.196	0.650	0	0
176	butanal	1.50E+04	E	< 3%	4.175	4.219	0	0.45	0.688	0.187	0.650	0	0
177	2-methylpropanal	2.11E+04	EP	< 3%	4.324	4.315	0	0.45	0.688	0.144	0.620	0	0
178	pentanal	4.58E+03	E	< 5%	3.661	3.747	0	0.45	0.829	0.163	0.650	0	0
179	heptanal	5.12E+02	E	< 5%	2.710	2.774	0	0.45	1.111	0.14	0.650	0	0
180	hexanal	1.45E+03	E	< 5%	3.162	3.267	0	0.45	0.970	0.146	0.650	0	0
181	octanal	1.54E+02	E	< 10%	2.187	2.251	0	0.45	1.252	0.16	0.650	0	0
182	nonanal	3.66E+01	E	< 5%	1.564	1.767	0	0.45	1.392	0.15	0.650	0	0
183	trans-crotonaldehyde	4.42E+03	EP	< 5%	3.645	3.910	0	0.5	0.645	0.387	0.800	0	0
184	o-tolualdehyde	6.34E+01	EP	< 25%	1.802	1.796	0	0.4	1.014	0.87	0.960	0	0
185	p-tolualdehyde	3.38E+01	P	< 5%	1.529	1.744	0	0.42	1.014	0.862	1.000	0	0
186	benzaldehyde	1.70E+02	E	< 5%	2.229	2.293	0	0.39	0.873	0.82	1.000	0	0
187	m-tolualdehyde	4.50E+01	EP	< 10%	1.653	1.816	0	0.42	1.014	0.84	0.970	0	0
188	acetone	3.08E+04	E	< 3%	4.488	4.652	0.04	0.49	0.547	0.179	0.700	0	0
189	2-butanone	1.23E+04	E	< 3%	4.090	4.167	0	0.51	0.688	0.166	0.700	0	0
190	3-pentanone	4.97E+03	E	< 3%	3.697	3.742	0	0.51	0.829	0.154	0.660	0	0
191	methyl isobutyl ketone	2.65E+03	E	< 10%	3.423	3.308	0	0.51	0.970	0.111	0.650	0	0
192	4-heptanone	7.71E+02	EP	< 10%	2.887	2.791	0	0.51	1.111	0.113	0.660	0	0
193	3-hexanone	1.85E+03	E	< 3%	3.268	3.264	0	0.51	0.970	0.136	0.660	0	0
194	2-pentanone	4.74E+03	E	< 3%	3.676	3.725	0	0.51	0.829	0.143	0.680	0	0
195	methyl isopropyl ketone	2.65E+03	E	< 10%	3.423	3.781	0	0.51	0.829	0.134	0.650	0	0
196	2-hexanone	1.55E+03	E	< 3%	3.191	3.233	0	0.51	0.970	0.136	0.680	0	0
197	2-heptanone	5.21E+02	E	< 3%	2.717	2.749	0	0.51	1.111	0.123	0.680	0	0
198	5-methyl-2-hexanone	6.93E+02	EP	< 3%	2.841	2.805	0	0.51	1.111	0.114	0.650	0	0
199	3,3-dimethyl-2-butanone	4.27E+03	E	< 10%	3.630	3.361	0	0.51	0.970	0.106	0.620	0	0
200	5-nonanone	7.93E+01	E	< 5%	1.899	1.806	0	0.51	1.392	0.103	0.660	0	0
201	2-nonanone	6.70E+01	EP	< 5%	1.826	1.757	0	0.51	1.392	0.119	0.680	0	0
202	cyclopentanone	1.51E+03	E	< 5%	3.178	3.569	0	0.52	0.720	0.373	0.860	0	0
203	cyclohexanone	5.52E+02	E	< 3%	2.742	3.034	0	0.56	0.861	0.403	0.860	0	0
204	2-octanone	1.87E+02	EP	< 10%	2.272	2.266	0	0.51	1.252	0.108	0.680	0	0
205	acetophenone	5.28E+01	E	< 3%	1.722	1.780	0	0.48	1.014	0.818	1.010	0	0
206	methyl formate	7.80E+04	E	< 1%	4.892	4.958	0	0.38	0.465	0.192	0.680	0	0
207	ethyl formate	3.26E+04	E	< 1%	4.513	4.542	0	0.38	0.606	0.146	0.660	0	0
208	n-propyl formate	1.10E+04	E	< 3%	4.041	4.104	0	0.38	0.747	0.132	0.630	0	0
209	n-butyl formate	3.85E+03	EP	< 3%	3.585	3.619	0	0.38	0.888	0.121	0.630	0	0
210	isobutyl formate	5.47E+03	E	< 3%	3.738	3.693	0	0.4	0.888	0.095	0.600	0	0
211	n-pentyl formate	1.19E+03	E	< 5%	3.076	3.143	0	0.38	1.028	0.101	0.630	0	0
212	methyl propionate	1.14E+04	E	< 1%	4.055	4.155	0	0.45	0.747	0.128	0.600	0	0
213	ethyl propionate	4.89E+03	E	< 1%	3.690	3.733	0	0.45	0.888	0.087	0.580	0	0
214	n-propyl propionate	1.86E+03	E	< 3%	3.270	3.287	0	0.45	1.028	0.07	0.560	0	0
215	n-propyl butanoate	7.77E+02	E	< 5%	2.890	2.811	0	0.45	1.169	0.05	0.560	0	0
216	methyl butanoate	4.29E+03	E	< 3%	3.633	3.681	0	0.45	0.888	0.106	0.600	0	0
217	ethyl butanoate	2.23E+03	E	< 3%	3.349	3.259	0	0.45	1.028	0.068	0.580	0	0
218	methyl acrylate	1.16E+04	E	< 3%	4.065	4.069	0	0.42	0.704	0.254	0.660	0	0
219	ethyl acrylate	5.00E+03	E	< 5%	3.699	3.649	0	0.42	0.845	0.212	0.640	0	0
220	n-butyl acrylate	7.27E+02	E	< 3%	2.861	2.724	0	0.42	1.126	0.177	0.620	0	0
221	methyl methacrylate	4.96E+03	E	< 5%	3.695	3.641	0	0.45	0.845	0.245	0.620	0	0
222	ethyl methacrylate	2.71E+03	EP	< 3%	3.433	3.224	0	0.45	0.986	0.2	0.600	0	0
223	isobutyl isobutyrate	5.95E+02	EP	< 5%	2.775	2.461	0	0.47	1.310	0	0.500	0	0
224	isobutyl methacrylate	4.84E+02	EP	< 5%	2.685	2.336	0	0.45	1.268	0.143	0.570	0	0
225	n-butyl methacrylate	2.77E+02	E	< 10%	2.442	2.258	0	0.45	1.268	0.171	0.600	0	0
226	methyl decanoate	4.95E+00	EP	< 10%	0.694	0.747	0	0.45	1.733	0.053	0.600	0	0
227	ethyl isobutyrate	3.38E+03	E	< 3%	3.529	3.344	0	0.47	1.028	0.034	0.550	0	0
228	isobutyl acrylate	9.42E+02	E	< 10%	2.974	2.794	0	0.42	1.126	0.156	0.590	0	0

Table S1. (cont.)

No.	Compound	P_{vap} (Pa)	Source	Error	Predicted log P_{vap}	log P_{vap}	A	B	V	E	S	λ	η
229	methyl acetate	2.86E+04	E	<1%	4.456	4.577	0	0.45	0.606	0.142	0.640	0	0
230	ethyl acetate	1.24E+04	E	<1%	4.094	4.150	0	0.45	0.747	0.106	0.620	0	0
231	n-propyl acetate	4.46E+03	E	<3%	3.649	3.697	0	0.45	0.888	0.092	0.600	0	0
232	n-butyl acetate	1.49E+03	E	<3%	3.174	3.225	0	0.45	1.028	0.071	0.600	0	0
233	isobutyl acetate	2.38E+03	E	<3%	3.376	3.293	0	0.47	1.028	0.052	0.570	0	0
234	isopentyl acetate	8.14E+02	E	<5%	2.910	2.794	0	0.47	1.169	0.051	0.570	0	0
235	allyl acetate	4.69E+03	EP	<5%	3.671	3.542	0	0.49	0.845	0.199	0.720	0	0
236	isopropyl acetate	8.05E+03	E	<3%	3.906	3.786	0	0.47	0.888	0.055	0.570	0	0
237	vinly acetate	1.51E+04	EP	<5%	4.179	4.136	0	0.43	0.704	0.223	0.640	0	0
238	n-pentyl acetate	5.63E+02	EP	<5%	2.751	2.729	0	0.45	1.169	0.067	0.600	0	0
239	benzyl acetate	2.11E+01	EP	<10%	1.323	1.029	0	0.65	1.214	0.789	1.060	0	0
240	n-hexyl acetate	1.76E+02	E	<5%	2.244	2.243	0	0.45	1.310	0.056	0.600	0	0
241	n-heptyl acetate	5.79E+01	E	<5%	1.762	1.750	0	0.45	1.451	0.05	0.600	0	0
242	n-octyl acetate	2.07E+01	EP	<10%	1.316	1.275	0	0.45	1.592	0.029	0.600	0	0
243	n-butyl benzoate	4.67E+00	E	<10%	0.670	0.570	0	0.46	1.495	0.668	0.800	0	0
244	methyl benzoate	5.03E+01	E	<5%	1.702	1.914	0	0.46	1.073	0.733	0.850	0	0
245	ethyl benzoate	3.81E+01	E	<5%	1.580	1.465	0	0.46	1.214	0.689	0.850	0	0
246	diethyl phthalate	6.64E-02	EP	<10%	-1.178	-1.180	0	0.88	1.711	0.729	1.400	0	0
247	dimethyl phthalate	4.56E-01	E	<10%	-0.341	-0.255	0	0.88	1.429	0.78	1.410	0	0
248	n-propyl benzoate	1.15E+01	EP	<10%	1.062	1.062	0	0.46	1.354	0.675	0.800	0	0
249	ethyl mercaptan	7.03E+04	E	<3%	4.847	4.912	0	0.24	0.554	0.392	0.350	0	0
250	n-propyl mercaptan	2.06E+04	E	<3%	4.313	4.421	0	0.24	0.695	0.385	0.350	0	0
251	n-hexyl mercaptan	5.96E+02	E	<5%	2.775	2.951	0	0.24	1.118	0.361	0.350	0	0
252	n-nonyl mercaptan	1.54E+01	E	<5%	1.187	1.469	0	0.24	1.540	0.347	0.350	0	0
253	n-octyl mercaptan	6.12E+01	E	<5%	1.787	1.962	0	0.24	1.399	0.353	0.350	0	0
254	n-pentyl mercaptan	1.84E+03	E	<3%	3.265	3.440	0	0.24	0.977	0.369	0.350	0	0
255	n-heptyl mercaptan	1.77E+02	E	<5%	2.247	2.458	0	0.24	1.258	0.357	0.350	0	0
256	n-butyl mercaptan	6.19E+03	E	<3%	3.791	3.925	0	0.24	0.836	0.382	0.350	0	0
257	phenyl mercaptan	2.02E+02	E	<3%	2.305	2.363	0.09	0.16	0.880	1	0.800	0	0
258	2-butyne	9.41E+04	E	<1%	4.974	5.027	0	0.15	0.586	0.261	0.300	0	0
259	1-pentyne	5.81E+04	EP	<3%	4.764	4.738	0.12	0.12	0.727	0.172	0.230	0	0
260	1-hexyne	1.77E+04	E	<5%	4.248	4.245	0.12	0.1	0.868	0.166	0.230	0	0
261	1-octyne	1.75E+03	EP	<5%	3.244	3.258	0.12	0.1	1.150	0.155	0.230	0	0
262	1-nonyne	4.94E+02	EP	<10%	2.694	2.764	0.12	0.1	1.291	0.15	0.230	0	0
263	phenylethyne	1.08E+03	EP	<10%	3.032	2.958	0.12	0.24	0.912	0.679	0.580	0	0
264	1-heptyne	5.56E+03	E	<5%	3.745	3.753	0.12	0.1	1.009	0.16	0.230	0	0
265	trimethylamine	2.16E+05	E	<5%	5.334	5.161	0	0.67	0.631	0.14	0.200	0	0
266	triethylamine	9.13E+03	E	<5%	3.960	3.783	0	0.79	1.054	0.101	0.150	0	0
267	quinoline	1.11E+01	E	<3%	1.047	1.211	0	0.54	1.044	1.268	0.970	0	0
268	pyridine	2.77E+03	E	<1%	3.443	3.459	0	0.52	0.675	0.631	0.840	0	0
269	N,N-dimethylaniline	9.72E+01	E	<3%	1.988	1.580	0	0.41	1.098	0.957	0.840	0	0
270	2-methylpyridine	1.51E+03	E	<3%	3.179	3.134	0	0.58	0.816	0.598	0.750	0	0
271	pyrimidine	2.25E+03	EP	<3%	3.352	3.389	0	0.7	0.634	0.606	1.000	0	0
272	2,6-dimethylpyridine	7.73E+02	E	<3%	2.888	2.700	0	0.63	0.957	0.607	0.700	0	0
273	3-methylpyridine	8.10E+02	E	<3%	2.908	3.004	0	0.54	0.816	0.631	0.810	0	0
274	4-methylpyridine	7.68E+02	E	<3%	2.885	2.990	0	0.54	0.816	0.63	0.820	0	0
275	N-methylpyrrole	2.92E+03	E	<5%	3.466	3.465	0	0.31	0.718	0.559	0.790	0	0
276	acetonitrile	1.21E+04	E	<3%	4.084	4.393	0.07	0.32	0.404	0.237	0.900	0.258	0
277	propionitrile	6.31E+03	E	<3%	3.800	3.981	0.02	0.36	0.545	0.162	0.900	0.258	0
278	n-butyronitrile	2.60E+03	E	<3%	3.415	3.451	0	0.36	0.686	0.188	0.900	0.258	0
279	isobutyronitrile	4.36E+03	EP	<5%	3.640	3.551	0	0.36	0.686	0.142	0.870	0.258	0
280	valeronitrile	9.72E+02	E	<3%	2.988	2.964	0	0.36	0.827	0.177	0.900	0.258	0
281	benzonitrile	8.64E+01	E	<5%	1.936	1.830	0	0.33	0.871	0.742	1.110	0.258	0
282	hexanenitrile	3.79E+02	E	<5%	2.579	2.477	0	0.36	0.968	0.166	0.900	0.258	0
283	nitromethane	4.81E+03	E	<5%	3.682	4.061	0.06	0.31	0.424	0.313	0.950	0.322	0
284	nitroethane	2.76E+03	E	<5%	3.441	3.611	0.02	0.33	0.565	0.27	0.950	0.322	0
285	2-nitropropane	2.28E+03	E	<5%	3.358	3.220	0	0.33	0.706	0.216	0.920	0.322	0
286	1-nitropropane	1.35E+03	E	<5%	3.129	3.144	0	0.31	0.706	0.242	0.950	0.322	0
287	1-nitrobutane	4.73E+02	E	<5%	2.675	2.662	0	0.29	0.847	0.227	0.950	0.322	0
288	nitrobenzene	3.35E+01	E	<5%	1.526	1.512	0	0.28	0.891	0.871	1.110	0.322	0
289	m-nitrotoluene	1.42E+01	E	<10%	1.153	1.024	0	0.25	1.032	0.874	1.100	0.322	0
290	o-nitrotoluene	1.99E+01	E	<5%	1.299	1.018	0	0.27	1.032	0.866	1.110	0.322	0

Table S1. (cont.)

No.	Compound	P_{vap} (Pa)	Source	Error	Predicted log P_{vap}	log P_{vap}	A	B	V	E	S	λ	η
291	benzene	1.26E+04	E	< 1%	4.102	4.131	0	0.14	0.716	0.61	0.520	-0.201	0
292	toluene	3.80E+03	E	< 3%	3.580	3.642	0	0.14	0.857	0.601	0.520	-0.201	0
293	o-xylene	8.86E+02	E	< 3%	2.948	3.009	0	0.16	0.998	0.663	0.560	-0.201	0
294	m-xylene	1.12E+03	E	< 3%	3.049	3.116	0	0.16	0.998	0.623	0.520	-0.201	0
295	p-xylene	1.17E+03	E	< 3%	3.068	3.128	0	0.16	0.998	0.613	0.520	-0.201	0
296	ethylbenzene	1.28E+03	E	< 3%	3.107	3.143	0	0.15	0.998	0.613	0.510	-0.201	0
297	o-ethyltoluene	3.39E+02	E	< 3%	2.530	2.505	0	0.18	1.139	0.68	0.550	-0.201	0
298	p-ethyltoluene	3.98E+02	E	< 3%	2.600	2.624	0	0.18	1.139	0.63	0.510	-0.201	0
299	1,2,3-trimethylbenzene	2.16E+02	E	< 3%	2.335	2.357	0	0.19	1.139	0.728	0.610	-0.201	0
300	1,2,4-trimethylbenzene	2.87E+02	E	< 3%	2.458	2.493	0	0.19	1.139	0.677	0.560	-0.201	0
301	cumene	6.09E+02	E	< 3%	2.784	2.687	0	0.16	1.139	0.602	0.490	-0.201	0
302	n-propylbenzene	4.64E+02	E	< 3%	2.666	2.669	0	0.15	1.139	0.604	0.500	-0.201	0
303	1,2,3,4-tetramethylbenzene	4.42E+01	EP	< 5%	1.645	1.705	0	0.19	1.280	0.794	0.660	-0.201	0
304	tert-butylbenzene	2.91E+02	E	< 3%	2.463	2.167	0	0.16	1.280	0.619	0.490	-0.201	0
305	isobutylbenzene	2.65E+02	E	< 3%	2.423	2.243	0	0.15	1.280	0.58	0.470	-0.201	0
306	n-butylbenzene	1.43E+02	E	< 3%	2.156	2.159	0	0.15	1.280	0.6	0.510	-0.201	0
307	n-pentylbenzene	4.39E+01	E	< 5%	1.643	1.666	0	0.15	1.421	0.594	0.510	-0.201	0
308	n-hexylbenzene	1.46E+01	EP	< 5%	1.164	1.185	0	0.15	1.562	0.591	0.500	-0.201	0
309	n-octylbenzene	1.49E+00	E	< 5%	0.174	0.230	0	0.15	1.844	0.579	0.480	-0.201	0
310	n-decylbenzene	1.51E-01	E	< 5%	-0.822	-0.751	0	0.15	2.125	0.579	0.470	-0.201	0
311	styrene	8.17E+02	E	< 1%	2.912	2.808	0	0.16	0.955	0.849	0.650	-0.201	0
312	?-methylstyrene	3.57E+02	EP	< 5%	2.552	2.321	0	0.19	1.096	0.851	0.640	-0.201	0
313	1-methylnaphthalene	1.00E+01	E	< 3%	1.002	1.077	0	0.2	1.226	1.344	0.900	-0.324	0
314	1-ethylnaphthalene	3.32E+00	E	< 5%	0.521	0.577	0	0.2	1.367	1.371	0.880	-0.324	0
315	2-ethylnaphthalene	4.23E+00	E	< 10%	0.627	0.593	0	0.2	1.367	1.331	0.900	-0.324	0
316	methylamine	3.53E+05	E	< 3%	5.548	5.603	0.16	0.58	0.349	0.25	0.350	0	0.61
317	ethylamine	1.40E+05	E	< 3%	5.145	5.109	0.16	0.61	0.490	0.236	0.350	0	0.61
318	allylamine	3.23E+04	P	< 5%	4.509	4.426	0.16	0.58	0.588	0.35	0.490	0	0.61
319	n-propylamine	4.13E+04	E	< 3%	4.616	4.622	0.16	0.61	0.631	0.225	0.350	0	0.61
320	isopropylamine	7.79E+04	E	< 3%	4.891	4.719	0.16	0.61	0.631	0.181	0.320	0	0.61
321	n-butylamine	1.24E+04	E	< 3%	4.093	4.123	0.16	0.61	0.772	0.224	0.350	0	0.61
322	isobutylamine	1.86E+04	E	< 3%	4.269	4.192	0.16	0.63	0.772	0.198	0.320	0	0.61
323	sec-butylamine	2.37E+04	EP	< 5%	4.374	4.225	0.16	0.63	0.772	0.17	0.320	0	0.61
324	tert-butylamine	4.95E+04	E	< 5%	4.695	4.300	0.16	0.71	0.772	0.121	0.290	0	0.61
325	n-pentylamine	4.00E+03	EP	< 3%	3.602	3.639	0.16	0.61	0.913	0.211	0.350	0	0.61
326	cyclohexylamine	1.34E+03	E	< 5%	3.127	3.082	0.16	0.58	0.945	0.326	0.560	0	0.61
327	benzylamine	8.82E+01	EP	< 5%	1.945	2.011	0.1	0.72	0.957	0.829	0.880	0	0.61
328	n-hexylamine	1.21E+03	E	< 5%	3.084	3.155	0.16	0.61	1.054	0.197	0.350	0	0.61
329	n-heptylamine	4.45E+02	E	< 5%	2.649	2.655	0.16	0.61	1.195	0.197	0.350	0	0.61
330	n-octylamine	1.34E+02	E	< 5%	2.128	2.171	0.16	0.61	1.335	0.187	0.350	0	0.61
331	methanol	1.68E+04	E	< 1%	4.226	4.334	0.43	0.47	0.308	0.278	0.440	0	2
332	ethanol	7.92E+03	E	< 1%	3.899	4.077	0.37	0.48	0.449	0.246	0.420	0	2
333	1-propanol	2.81E+03	E	< 3%	3.449	3.589	0.37	0.48	0.590	0.236	0.420	0	2
334	1-butanol	8.93E+02	E	< 3%	2.951	3.104	0.37	0.48	0.731	0.224	0.420	0	2
335	1-pentanol	3.32E+02	EP	< 3%	2.521	2.610	0.37	0.48	0.872	0.219	0.420	0	2
336	1-hexanol	1.03E+02	EP	< 5%	2.014	2.120	0.37	0.48	1.013	0.21	0.420	0	2
337	1-heptanol	2.75E+01	EP	< 3%	1.439	1.619	0.37	0.48	1.154	0.211	0.420	0	2
338	1-octanol	1.06E+01	E	< 3%	1.024	1.134	0.37	0.48	1.295	0.199	0.420	0	2
339	1-nonanol	3.14E+00	E	< 3%	0.497	0.644	0.37	0.48	1.435	0.193	0.420	0	2
340	1-decanol	1.14E+00	E	< 3%	0.056	0.147	0.37	0.48	1.576	0.191	0.420	0	2
341	1-undecanol	4.26E-01	E	< 5%	-0.371	-0.341	0.37	0.48	1.717	0.181	0.420	0	2
342	1-dodecanol	1.18E-01	E	< 5%	-0.928	-0.834	0.37	0.48	1.858	0.175	0.420	0	2
343	allyl alcohol	3.39E+03	EP	< 5%	3.530	3.523	0.38	0.48	0.547	0.342	0.460	0	2
344	2-chloroethanol	9.57E+02	E	< 5%	2.981	2.535	0.47	0.57	0.572	0.419	0.590	0	2
345	2-methyl-1-propanol	1.40E+03	EP	< 3%	3.146	3.157	0.37	0.48	0.731	0.217	0.390	0	2
346	2-methyl-1-butanol	4.86E+02	E	< 3%	2.687	2.655	0.37	0.48	0.872	0.219	0.390	0	2
347	3-methyl-1-butanol	4.27E+02	E	< 5%	2.630	2.687	0.37	0.48	0.872	0.192	0.390	0	2
348	benzyl alcohol	1.27E+01	E	< 10%	1.102	1.037	0.33	0.56	0.916	0.803	0.870	0	2
349	dimethylamine	2.03E+05	E	< 3%	5.308	5.451	0.08	0.66	0.490	0.189	0.300	0	0
350	diethylamine	3.14E+04	E	< 3%	4.497	4.493	0.08	0.69	0.772	0.154	0.300	0	0
351	piperidine	4.28E+03	E	< 3%	3.632	3.822	0.1	0.69	0.804	0.422	0.460	0	0
352	di-n-propylamine	3.61E+03	EP	< 10%	3.558	3.528	0.08	0.69	1.054	0.124	0.300	0	0

Table S1. (cont.)

No.	Compound	P_{vap} (Pa)	Source	Error	Predicted log P_{vap}	log P_{vap}	A	B	V	E	S	λ	η
353	diisopropylamine	1.06E+04	E	<5%	4.024	3.702	0.08	0.73	1.054	0.523	0.240	0	0
354	di-n-butylamine	3.65E+02	E	<3%	2.562	2.552	0.08	0.69	1.335	0.107	0.300	0	0
355	2-propanol	6.05E+03	EP	<3%	3.782	4.034	0.33	0.56	0.590	0.212	0.360	0	1.43
356	2-butanol	2.41E+03	E	<3%	3.383	3.528	0.33	0.56	0.731	0.217	0.360	0	1.43
357	3-methyl-2-butanol	1.21E+03	E	<5%	3.082	3.101	0.33	0.56	0.872	0.194	0.330	0	1.43
358	3-pentanol	1.09E+03	E	<5%	3.037	3.027	0.33	0.56	0.872	0.218	0.360	0	1.43
359	2-pentanol	8.22E+02	E	<3%	2.915	3.054	0.33	0.56	0.872	0.195	0.360	0	1.43
360	4-methyl-2-pentanol	7.02E+02	E	<5%	2.846	2.633	0.33	0.56	1.013	0.167	0.330	0	1.43
361	2-hexanol	3.34E+02	E	<5%	2.524	2.564	0.33	0.56	1.013	0.187	0.360	0	1.43
362	2-heptanol	1.27E+02	EP	<5%	2.103	2.063	0.33	0.56	1.154	0.188	0.360	0	1.43
363	2-octanol	3.23E+01	E	<3%	1.509	1.598	0.33	0.56	1.295	0.158	0.360	0	1.43
364	1-phenylethanol	2.37E+01	E	<5%	1.375	0.929	0.3	0.66	1.057	0.784	0.830	0	1.43
365	pyrrole	1.10E+03	E	<3%	3.040	3.452	0.41	0.29	0.577	0.613	0.730	0	1.27
366	aniline	9.01E+01	E	<3%	1.955	1.912	0.26	0.41	0.816	0.955	0.960	0	1.27
367	o-chloroaniline	3.30E+01	E	<5%	1.519	1.580	0.25	0.31	0.939	1.033	0.920	0	1.27
368	m-chloroaniline	8.79E+00	E	<5%	0.944	1.225	0.3	0.3	0.939	1.053	1.100	0	1.27
369	N-methylaniline	5.98E+01	E	<3%	1.776	1.665	0.17	0.43	0.957	0.948	0.900	0	1.27
370	o-toluidine	3.47E+01	E	<5%	1.540	1.475	0.23	0.45	0.957	0.966	0.920	0	1.27
371	m-toluidine	2.58E+01	E	<5%	1.412	1.453	0.23	0.45	0.957	0.946	0.950	0	1.27
372	2-methyl-2-propanol	5.58E+03	E	<3%	3.747	3.745	0.31	0.6	0.731	0.18	0.310	0	1.27
373	2-methyl-2-butanol	2.23E+03	E	<3%	3.347	3.377	0.32	0.49	0.872	0.194	0.300	0	1.27
374	m-cresol	1.85E+01	E	<3%	1.267	1.438	0.57	0.34	0.916	0.822	0.880	0	1.27
375	m-ethylphenol	6.98E+00	E	<5%	0.844	0.862	0.55	0.37	1.057	0.81	0.910	0	1.27
376	o-ethylphenol	2.07E+01	E	<5%	1.317	0.995	0.52	0.37	1.057	0.831	0.840	0	1.27

Explanation of column headings: Values of Pvap are calculated from DIPPR equation 101, using the constants given for a specific compound. The source of the constants is experimental (E), predicted (P), or a combination of the two (EP). The error is the maximum percent error of the resulting Pvap values as determined by DIPPR. Predicted log Pvap is the value of log Pvap calculated using equation 6 and the solute parameters *A, B, V, E, S,* λ, and η. The sources of the parameters *A, B, V, E,* and *S* are given in the text, and the values of λ, and η are taken from the manuscript.

Table S2. Solute parameters estimated from molecular structure*

Compound Class	***A***	***B***	***S***
Alkane	0	0	0
Cycloalkane	0	0	0.13
Acyclic Alkene	0	0.08	0.12
Cycloalkene	0	0.03	0.08
Conjugated Diene	0	0.11	0.23
Alkylbenzene (note λ also)	0	0.16	0.53
Dialkyl Sulfide	0	0.30	0.38
Dialkyl Disulfide	0	0.28	0.46
Dialkyl Ether	0	0.44	0.24
Aliphatic Aldehyde	0	0.44	0.65
Aliphatic Ketone	0	0.51	0.67
Aliphatic Ester	0	0.44	0.60
Aliphatic Nitrile (note λ also)	0.02	0.35	4.90
Alkylmercaptan	0	0.24	0.35
Terminal Alkyne	0.12	0.12	0.23
Internal Alkyne	0	0.15	0.00
Primary Aliphatic Amine (note η also)	0.16	0.62	0.35
Secondary Aliphatic Amine	0.08	0.69	0.29
Tertiary Aliphatic Amine	0	0.73	0.18
Primary Alcohol (note η also)	0.37	0.48	0.42
Secondary Alcohol(note η also)	0.33	0.56	0.35
Tertiary Alcohol (note η also)	0.32	0.55	0.31
Alkylnaphthalene (note λ also)	0	0.20	0.89

*E values for molecules with a particular functional group tend to decrease with increasing alkyl substitution because the difference between the compound´s index of refraction and the index of refraction of an alkane with the same molecular volume tends to decrease as the compound becomes more alkane-like. Thus E values may be interpolated from values of homologous compounds in Table S1 above if a sufficient range of values is available. This was done for the compounds in Table S3 except for the higher molecular weight trialkylamines, for which E values were calculated as indicated in Lima, G. A. R. Ph.D. Thesis, University of São Paulo, Brazil, 2000.

Table S3. Solute parameters and log P_{vap} values used to prepare Figure 5

No.	Compound	P_{vap} (Pa)	Source	Error	A	B	V	E	S+λ	η*A*B	log P_{vap}	Predicted log P_{vap}
1	propylcyclopentane	1.647E+03	EP	< 3%	0	0	1.127	0.225	0.100	0	3.217	3.456
2	5-methyl-1-hexene	1.034E+04	P	< 5%	0	0.078	1.052	0.092	0.080	0	4.015	3.908
3	trans-2-pentene	6.743E+04	E	< 1%	0	0.078	0.770	0.092	0.080	0	4.829	4.907
4	2-ethyl-1-butene	2.338E+04	E	< 3%	0	0.078	0.911	0.092	0.080	0	4.369	4.407
5	2,4,4-trimethyl-2-pentene	4.786E+03	E	< 3%	0	0.078	1.193	0.092	0.080	0	3.680	3.408
6	1-tridecene	7.334E+00	E	< 3%	0	0.078	1.897	0.092	0.080	0	0.865	0.912
7	6-methyl-1-heptene	3.305E+03	P	< 5%	0	0.078	1.193	0.092	0.080	0	3.519	3.408
8	1-heptadecene	6.924E-02	E	< 5%	0	0.078	2.461	0.092	0.080	0	-1.160	-1.086
9	trans-1,3-pentadiene	5.482E+04	E	< 1%	0	0.113	0.727	0.352	0.230	0	4.739	4.528
10	trans,trans-2,4-hexadiene	1.171E+04	E	< 1%	0	0.113	0.868	0.352	0.230	0	4.069	4.028
11	1,2-dichlorobutane	2.165E+03	EP	< 5%	0.1	0.11	0.917	0.680	0.220	0	3.336	3.488
12	2,3-dichlorobutane	2.701E+03	EP	< 10%	0.1	0.11	0.917	0.680	0.220	0	3.431	3.488
13	isopropyl iodide	9.493E+03	E	< 5%	0	0.15	0.654	0.634	0.400	0	3.977	4.201
14	m-ethyltoluene	4.243E+02	E	< 3%	0	0.16	1.139	0.640	0.316	0	2.628	2.602
15	sec-butylbenzene	2.241E+02	E	< 3%	0	0.16	1.280	0.640	0.316	0	2.350	2.102
16	m-cymene	2.322E+02	E	< 3%	0	0.16	1.280	0.640	0.316	0	2.366	2.102
17	m-diethylbenzene	1.604E+02	E	< 3%	0	0.16	1.280	0.640	0.316	0	2.205	2.102
18	p-diisopropylbenzene	3.281E+01	E	< 3%	0	0.16	1.562	0.640	0.316	0	1.516	1.104
19	heptylbenzene	4.803E+00	EP	< 5%	0	0.16	1.703	0.640	0.316	0	0.681	0.604
20	undecylbenzene	4.596E-02	E	< 3%	0	0.16	2.266	0.640	0.316	0	-1.338	-1.393
21	methyl propyl sulfide	6.786E+03	E	< 3%	0	0.3025	0.836	0.381	0.380	0	3.832	3.880
22	ethyl octyl sulfide	1.213E+01	E	< 3%	0	0.3025	1.681	0.381	0.380	0	1.084	0.884
23	dipropyl disulfide	1.039E+02	E	< 3%	0	0.28	1.281	0.683	0.460	0	2.017	1.829
24	methyl butyl sulfide	2.079E+03	E	< 3%	0	0.3025	0.977	0.381	0.380	0	3.318	3.381
25	di-sec-butyl ether	2.144E+03	EP	< 5%	0	0.437	1.295	0.030	0.243	0	3.331	2.871
26	methyl ethyl ether	1.959E+05	E	< 5%	0	0.437	0.590	0.030	0.243	0	5.292	5.368
27	butyl isopropyl ether	3.462E+03	EP	< 5%	0	0.437	1.154	0.030	0.243	0	3.539	3.371
28	dihexyl ether	6.144E+00	EP	< 5%	0	0.437	1.858	0.030	0.243	0	0.788	0.874
29	methyl butyl ether	1.829E+04	EP	< 5%	0	0.437	0.872	0.030	0.243	0	4.262	4.369
30	ethyl propyl ether	2.407E+04	E	< 5%	0	0.437	0.872	0.030	0.243	0	4.381	4.369
31	dipentyl ether	1.142E+02	EP	< 5%	0	0.437	1.576	0.030	0.243	0	2.058	1.873
32	methyl pentyl ether	5.694E+03	EP	< 5%	0	0.437	1.013	0.030	0.243	0	3.755	3.870
33	butyl ethyl ether	7.367E+03	EP	< 3%	0	0.437	1.013	0.030	0.243	0	3.867	3.870
34	ethyl hexyl ether	6.431E+02	EP	< 10%	0	0.437	1.295	0.030	0.243	0	2.808	2.871
35	2-ethylhexanal	2.615E+02	EP	< 5%	0	0.438	1.252	0.171	0.654	0	2.417	2.234
36	3-methylhexanal	8.033E+02	EP	< 5%	0	0.438	1.111	0.171	0.654	0	2.905	2.733
37	decanal	1.271E+01	E	< 5%	0	0.438	1.533	0.171	0.654	0	1.104	1.235
38	dodecanal	1.649E+00	E	< 5%	0	0.438	1.815	0.171	0.654	0	0.217	0.236
39	3-methyl-2-pentanone	2.568E+03	E	< 5%	0	0.509	0.970	0.130	0.667	0	3.410	3.261
40	3-heptanone	5.619E+02	E	< 10%	0	0.509	1.111	0.130	0.667	0	2.750	2.762
41	ethyl isopropyl ketone	2.733E+03	E	< 10%	0	0.509	0.970	0.130	0.667	0	3.437	3.261
42	octyl formate	8.125E+01	EP	< 5%	0	0.438	1.451	0.093	0.597	0	1.910	1.704
43	nonyl formate	2.278E+01	EP	< 10%	0	0.438	1.592	0.093	0.597	0	1.358	1.205
44	sec-butyl acetate	2.961E+03	EP	< 5%	0	0.438	1.028	0.093	0.597	0	3.471	3.202
45	butyl propionate	5.970E+02	EP	< 5%	0	0.438	1.169	0.093	0.597	0	2.776	2.703
46	propyl isobutyrate	8.874E+02	EP	< 5%	0	0.438	1.169	0.093	0.597	0	2.948	2.703
47	butyl valerate	7.847E+01	EP	< 10%	0	0.438	1.451	0.093	0.597	0	1.895	1.704
48	ethyl isovalerate	1.073E+03	EP	< 5%	0	0.438	1.169	0.093	0.597	0	3.030	2.703
49	nonyl acetate	6.663E+00	EP	< 10%	0	0.438	1.733	0.093	0.597	0	0.824	0.705
50	decyl acetate	1.553E+00	E	< 25%	0	0.438	1.874	0.093	0.597	0	0.191	0.206
51	hexyl formate	3.559E+02	EP	< 5%	0	0.438	1.169	0.093	0.597	0	2.551	2.703
52	heptyl formate	1.699E+02	EP	< 5%	0	0.438	1.310	0.093	0.597	0	2.230	2.203
53	t-butanethiol	2.416E+04	E	< 3%	0	0.24	0.836	0.372	0.350	0	4.383	3.937
54	2-methylpropanethiol	9.275E+03	E	< 3%	0	0.24	0.836	0.372	0.350	0	3.967	3.937
55	hexanethiol	5.961E+02	E	< 5%	0	0.24	1.118	0.372	0.350	0	2.775	2.938
56	2-propanethiol	3.694E+04	E	< 3%	0	0.24	0.695	0.372	0.350	0	4.567	4.436
57	3-hexyne	1.213E+04	EP	< 5%	0	0.15	0.868	0.261	0.300	0	4.084	4.028
58	2-hexyne	1.067E+04	EP	< 3%	0	0.15	0.868	0.261	0.300	0	4.028	4.028
59	1-decyne	1.651E+02	EP	< 10%	0.12	0.117	1.432	0.166	0.233	0	2.218	2.243
60	nonylamine	4.345E+01	E	< 5%	0.16	0.616	1.477	0.208	0.354	0.06	1.638	1.639
61	decylamine	1.329E+01	E	< 5%	0.16	0.616	1.617	0.208	0.354	0.06	1.123	1.140
62	dipentylamine	2.042E+01	EP	< 10%	0.08	0.692	1.617	0.125	0.288	0	1.310	1.548

Table S3. (cont.)

No.	Compound	P_{vap} (Pa)	Source	Error	A	B	V	E	S+λ	η*A*B	log P_{vap}	Predicted log P_{vap}
63	2-methyl-2-butanamine	1.349E+04	EP	< 5%	0	0.73	0.913	0.121	0.354	0	4.130	3.950
64	butyldimethylamine	7.062E+03	EP	< 10%	0	0.73	1.054	0.121	0.180	0	3.849	3.716
65	tributylamine	1.244E+01	EP	< 5%	0	0.73	1.899	0.020	0.180	0	1.095	0.836
66	2-methylpentanol	1.951E+02	E	< 5%	0.37	0.48	1.013	0.210	0.420	0.355	2.290	2.120
67	3-methylpentanol	1.285E+02	E	< 5%	0.37	0.48	1.013	0.210	0.420	0.355	2.109	2.120
68	2-methylhexanol	8.598E+01	EP	< 5%	0.37	0.48	1.154	0.208	0.420	0.355	1.934	1.625
69	5-methylhexanol	5.143E+01	EP	< 10%	0.37	0.48	1.154	0.211	0.420	0.355	1.711	1.619
70	8-methylnonanol	2.753E+00	EP	< 5%	0.37	0.48	1.576	0.191	0.420	0.355	0.440	0.147
71	2-nonanol	1.718E+01	EP	< 10%	0.33	0.56	1.435	0.193	0.420	0.259	1.235	0.989
72	3-methyl-3-pentanol	1.334E+03	E	< 10%	0.32	0.49	1.013	0.194	0.300	0.188	3.125	2.920
73	nonylphenol	3.143E-03	EP	< 10%	0.55	0.37	2.043	0.810	0.910	0.244	-2.503	-2.579
74	1-butylnaphthalene	4.378E-01	EP	< 10%	0	0.2	1.649	1.371	0.541	0	-0.359	-0.401
75	1-propylnaphthalene	1.760E+00	E	< 10%	0	0.2	1.508	1.371	0.541	0	0.246	0.099
76	1-pentylnaphthalene	1.606E-01	EP	< 10%	0	0.2	1.790	1.371	0.541	0	-0.794	-0.900

Table S4. Statistical data for LSER correlations

Equations 2, 4, 5, and 6 are reproduced below. The uncertainties shown for each intercept and coefficient are the standard deviations of those values. Below each equation are shown the partial *F* values for the parameter immediately above the value indicated.

Equation 2

$$\log P_{vap} = (7.78 \pm 0.04) - (3.45 \pm 0.03)\,V - (0.93 \pm 0.04)\,E - (1.70 \pm 0.04)\,S$$

Partial *F* values for the coefficients: 10497 456 1506

Equation 4

$$\log P_{vap} = (7.86 \pm 0.03) - (3.54 \pm 0.03)\,V - (1.17 \pm 0.03)\,E - (1.52 \pm 0.03)\,(S + \lambda)$$

Partial *F* values for the coefficients: 18236 1474 2764

Equation 5

$$\log P_{vap} = (7.92 \pm 0.04) - (3.58 \pm 0.03)\,V - (1.15 \pm 0.04)\,E - (1.53 \pm 0.04)\,(S + \lambda) - (5.75 \pm 0.17)\,(A \times B)$$

Partial *F* values for the coefficients: 13654 948 1784 1098

Equation 6

$$\log P_{vap} = (7.86 \pm 0.03) - (3.54 \pm 0.02)\,V - (1.17 \pm 0.03)\,E - (1.52 \pm 0.03)\,(S + \lambda) - (3.64 \pm 0.08)\,(\eta \times A \times B)$$

Partial F values for the coefficients: 21270 1533 2782 1954

Table S5. Correlation matrix for solute parameters

The following table shows the cross-correlation of the solute parameters for all 376 compounds in the data set used to generate equation 6:

	A	B	V	E	S
A	1				
B	0.370683	1			
V	-0.14024	-0.21814	1		
E	0.095105	0.083291	-0.17908	1	
S	0.108824	0.553608	-0.28583	0.658822	1