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SUPPORTING INFORMATION

QUANTUM CHEMICAL CALCULATION OF THE VAPOR PRESSURE OF VOLATILE AND SEMI VOLATILE ORGANIC COMPOUNDS

Marcel Stahn[1], Stefan Grimme[1], Tunga Salthammer[2*], Uwe Hohm[3], Wolf-Ulrich Palm[4]

1) Mulliken Center for Theoretical Chemistry, Institute for Physical and Theoretical Chemistry, University of Bonn, 53115 Bonn, Germany

2) Department of Material Analysis and Indoor Chemistry, Fraunhofer WKI, 38108 Braunschweig, Germany

3) Institute of Physical and Theoretical Chemistry, University of Braunschweig – Institute of Technology, 38106 Braunschweig, Germany

4) Institute of Sustainable and Environmental Chemistry, Leuphana University Lüneburg, 21335 Lüneburg, Germany

*) Corresponding author:

Prof. Dr. Tunga Salthammer

Email: tunga.salthammer@wki.fraunhofer.de

Fundamentals of vapor pressure thermodynamics

As displayed in Figure 1 (see main text) two phases of a pure substance at equilibrium are considered. In this pressure-temperature diagram the functional relationship between the equilibrium pressure P and the equilibrium temperature T is given by the Clapeyron equation (S1).

$$\frac{dP}{dT} = \frac{\Delta_{trs}S}{\Delta_{trs}V} = \frac{\Delta_{trs}H}{T \cdot \Delta_{trs}V} \tag{S1}$$

$\Delta_{trs}S$, $\Delta_{trs}H$, and $\Delta_{trs}V$ are the changes in molar entropy, molar enthalpy, and molar volume, respectively, upon phase transition. In the following we only consider the equilibrium between the condensed phase and the vapor phase. Assuming ideal gas behavior and neglecting the molar volume of the condensed phase, $\Delta_{trs}V = \Delta_{vap}V \approx V_{m,g} \approx P/(RT)$, the Clausius-Clapeyron equation (S2) results,

$$\frac{dlnP}{dT} = \frac{\Delta_{vap}H}{R \cdot T^2} \tag{S2}$$

where R is the molar gas constant and $\Delta_{vap}H$ is the molar enthalpy of vaporization. Equation (S2) can be used for extrapolation of vapor pressure data. Under the assumption that $\Delta_{vap}H$ is constant in the interval between T_1 and T_2, the vapor pressure $P_1(T_1)$ given at a temperature $T_{fus} < T_1$ can be used to calculate $P_2(T_2)$ for a temperature $T_{fus} < T_2$, T_{fus} being the melting point. If, however, $T_2 < T_{fus} < T_1$ use of $P_1(T_1)$ and $\Delta_{vap}H$ = const. in equation (2) will result in the vapor pressure $P_2(T_2)$ of the sub-cooled liquid (see Figure 1 in main text).

Table S1: Conversion of units for pressure.

1 Pa	---	$9.8692 \cdot 10^{-6}$ atm	$1.0 \cdot 10^{-5}$ bar	0.0075 Torr
1 atm	101,325 Pa	---	1.01325 bar	760 Torr
1 bar	100,000 Pa	0.98692 atm	---	750.06376 Torr
1 Torr (= 1 mm Hg)	133.322 Pa	0.00132 atm	0.00133 bar	---

Conversion from vapor pressure P_L of the sub-cooled liquid to the saturation concentration C_0 according to the ideal gas law

$$C_0 = \frac{m}{V} = \frac{P_L \cdot MW}{R \cdot T}$$

For C_0 in µg/m³, T = 298.15 K, R = 8.314 J/(K·mol), P_L in Pa, and MW in g/mol:

$$C_0 \left(\frac{\mu g}{m^3}\right) = P_L(Pa) \cdot MW \left(\frac{g}{mol}\right) \cdot 403.42$$

Conversion of energies between Calories and Joule

Please note that in quantum mechanical publications, the use of the unit "Calorie" for energies is still common and dominant.

1 cal = 4.1868 J 1 J = 0.2388 cal

SMILES

The SMILES (Simplified Molecular-Input Line-Entry System) notation for the selected isomer (see Tables S3 and S5) was taken from PubChem (https://pubchem.ncbi.nlm.nih.gov/).

Table S2: Literature data of the reference compounds (SL = subcooled liquid, DCP = decomposition at higher temperatures).

Compound	Abbr.	CAS	Density kg/m³	MP (°C)	BP (°C)	P_L (Pa)	Remark	$\Delta_{vap}H$ (kJ/mol)	Ref.
n-Decane	C10	124-18-5	730	-29.7	174.1	182	298.15 K	51.4	[1]
n-Hexadecane	C16	544-76-3	773	18.2	286.9	0.19	298.15 K	81.4	[2]
N-Tridecylbenzene	TDB	123-02-4	881	10.0	346.0	0.007	298.15 K	90.4	[3, 4]
3-Cresol	3CR	108-39-4	1034	12.2	202	18.27	298.05 K	61.8±1.0	[5]
Naphthalene	NAP	91-20-3	1162	80.3	217.9	37.0	298.15 K **(SL)**	56.1	[6]
Anthracene	ANT	120-12-7	1240	215.8	339.9	0.072	298.15 K **(SL)**	72.4	[6]
Fluoranthene	FLU	206-44-0	1252	110.2	384	$6.0 \cdot 10^{-3}$	298.15 K **(SL)**	79.3	[6]
2-Butoxy ethanol	EGBE	111-76-2	902	-75	171	115	298 K	56.6	[7, 8]
1-Undecanol	UDC	112-42-5	835	19	243	0.2383	293.18 K	85.0	[9]
Oleyl alcohol	OA	143-28-2	849	7	>300	$3.7 \cdot 10^{-4}$	298.15 K	101.2 [4]	[10]
Glycerol	GLY	56-81-5	1261	18.1	290.0	0.0249	298.75	86.76±0.70	[11]
Benzophenone	BP	119-61-9	1085	48.5	305.4	0.157	298.48 K **(SL)**	77.1	[12, 13]
Benzophenone-3	BP-3	131-57-7	1320	64	315	$4.8 \cdot 10^{-3}$	298.15 K **(SL)**	76.3	[13]
Homosalate	HS	118-56-9	1045	<-20	341	$1.1 \cdot 10^{-2}$	298.15 K	95.3	[13]
Dimethyl phthalate	DMP	131-11-3	1190	5.5	283.7	0.304	298.15 K	77.0	[14]
Diethyl phthalate	DEP	84-66-2	1120	-40.5	295	0.099	298.15 K	82.1	[15]
Di-n-butyl phthalate	DnBP	84-74-2	1049	-35	340	$4.3 \cdot 10^{-3}$	298.15 K	95.2	[16]
Butyl benzyl phthalate	BBzP	85-68-7	1120	-35.0	370	$2.0 \cdot 10^{-4}$	298.15 K	106.2	[16]
Dihexyl phthalate [a)]	DHP	84-75-3	995	-58	350	*($1.1 \cdot 10^{-3}$)*	298.15 K	111.2 [4]	[17]
Di-(2-ethylhexyl) phthalate	DEHP	117-81-7	990	-55.0	384.0	$1.6 \cdot 10^{-5}$	298 K	116.7	[16, 18]
Di-(2-ethylhexyl) terephthalate	DEHTP	6422-86-2	982	-48.0	383	$5.4 \cdot 10^{-6}$	298.15 K	123.3	[16]
Methyl palmitoleate	MP	1120-25-8	875	0	>250	$5.1 \cdot 10^{-3}$	298.15 K	96.4 [17]	[19]

Glutaric acid	GA	110-94-1	1424	98	303	$1.0 \cdot 10^{-3}$	298 K **(SL)**	118	[20]
Pimelic acid	PA	111-16-0	1280	106	>400	$2.2 \cdot 10^{-4}$	298 K **(SL)**	108	[20]
Tris-(2-ethylhexyl) phosphate	TEHP	78-42-2	926	-74	DCP	$3.0 \cdot 10^{-5}$	298.15 K	106	[13]
Tris-(2-butoxyethyl) phosphate	TBOEP	78-51-3	1020	-70	>400	$6.8 \cdot 10^{-5}$	298.15 K	103	[13, 21]
2,4,4'-Trichlorobiphenyl	PCB-28	7012-37-5	1400	58	207	$2.7 \cdot 10^{-2}$	298.15 K **(SL)**	77.1	[22]
2,2',4,5,5'-Pentachlorobiphenyl	PCB-101	37680-73-2	1522	77	>400	$2.5 \cdot 10^{-3}$	298.15 K **(SL)**	86.2	[22]
2,4,5,2‘,4‘,5‘-Hexachlorobiphenyl	PCB-153	35065-27-1	(1000)[b)]	103	>400	$6.1 \cdot 10^{-4}$	298.15 K **(SL)**	91.8	[22]
2,2',3,4,4',5,5'-Heptachlorobiphenyl	PCB-180	35065-29-3	1640	112	>400	$1.1 \cdot 10^{-4}$	298.15 K **(SL)**	94.1	[22]
1,10-Dichlorodecane	C10Cl2	2162-98-3	994	15.6	284.3	0.50	298.15 K	67.3	[23]
1,2,11,12-Tetrachlorododecane	C12Cl4	210115-98-3	1100	-	354.6	$3.5 \cdot 10^{-3}$	298.15 K **(SL)**	81.9	[23]
2,2′,4,4′-Tetrabromodiphenyl ether	BDE-47	5436-43-1	2161	84.0	DCP	$3.2 \cdot 10^{-4}$	298.15 K **(SL)**	92.0	[24]
2,2′,4,4′,5-Pentabromodiphenyl ether	BDE-99	60348-60-9	2250	92.5	DCP	$6.8 \cdot 10^{-5}$	298.15 K **(SL)**	100.3	[24]
1,2,3,4,5-Pentabromo-6-ethyl benzene	PBEB	85-22-3	(1000)[b)]	138	-	$2.9 \cdot 10^{-3}$	298.15 K **(SL)**	78.3	[13]
Dodecamethylcyclohexasiloxane	D6	540-97-6	967	-3.0	245	2.26	298.15 K	65	[25]
Hexadecamethylheptasiloxane	L7	541-01-5	901	-78.0	286.8	$7.4 \cdot 10^{-2}$	298.15 K	89	[25]
Octadecamethyloctasiloxane	L8	556-69-4	913	-63	311.6	$9.3 \cdot 10^{-3}$	298.15 K	98	[25]
pp‘-DDT	DDT	50-29-3	980	109	260	$4.8 \cdot 10^{-4}$	298.15 K **(SL)**	89.3	[13, 26]
Diazinon	DZN	333-41-5	1117	<25	-	$5.9 \cdot 10^{-3}$	298.15 K	87.5	[27, 28]
Fipronil	FIP	120068-37-3	1477	200	DCP	$1.9 \cdot 10^{-6}$	298.15 K **(SL)**	85	[27]

a) The published reference value for DHP is doubtful.
b) Default value – density not available

Table S3: Log P_L values of the reference compounds (see Table S1), calculated SPARC and LFER values (298 K), COSMO values from the literature (SL = subcooled liquid).

Compound	Abbr.	CAS	log P_L (Reference) (Pa)	log P_L (SPARC) [a] (Pa)	log P_L (LFER) [b] (Pa)	log P_L (COSMO-RS) (Pa)	Remark
n-Decane	C10	124-18-5	2.26	2.28	2.34		298.15
n-Hexadecane	C16	544-76-3	-0.72	-0.82	-0.41		298.15 K
N-Tridecylbenzene	TDB	123-02-4	-2.15	-2.53	-1.93		298.15 K
3-Cresol	3CR	108-39-4	1.26	1.62	1.28		298.05
Naphthalene	NAP	91-20-3	1.57	1.52	1.54	1.84 [29]	298.15 K **(SL)**
Anthracene	ANT	120-12-7	-1.14	-1.31	-1.02	-0.37 [29]	298.15 K **(SL)**
Fluoranthene	FLU	206-44-0	-2.22	-2.07	-2.40	-1.33 [29]	298.15 K **(SL)**
2-Butoxy ethanol	EGBE	111-76-2	2.06	1.70	1.66		298 K
1-Undecanol	UDC	112-42-5	-0.36	-0.64	0.01		298.18 K
Oleyl alcohol	OA	143-28-2	-3.43	-4.15	-3.50		298.15 K
Glycerol	GLY	56-81-5	-1.60	-1.26	-0.72		298.75
Benzophenone	BP	119-61-9	-0.80	-0.74	-0.58		298.48 K **(SL)**
Benzophenone-3	BP-3	131-57-7	-2.32	-3.79	-2.53		298.15 K **(SL)**
Homosalate	HS	118-56-9	-1.96	-2.44	-1.72		298.15 K
Dimethyl phthalate	DMP	131-11-3	-0.52	-1.25	0.26		298.15 K
Diethyl phthalate	DEP	84-66-2	-1.00	-1.82	-0.40		298.15 K
Di-n-butyl phthalate	DnBP	84-74-2	-2.37	-3.47	-2.18		298.15 K
Butyl benzyl phthalate	BBzP	85-68-7	-3.70	-5.47	-4.12		298.15 K
Dihexyl phthalate [d]	DHP	84-75-3	*(-2.96)*	-5.40	-4.11		298.15 K
Di-(2-ethylhexyl) phthalate	DEHP	117-81-7	-4.80	-6.85	-5.48		298 K

Di-(2-ethylhexyl) terephthalate	DEHTP	6422-86-2	-5.27	-6.44	-4.96		298.15 K
Methyl palmitoleate	MP	1120-25-8	-2.29	-1.95	-1.59		298.15 K
Glutaric acid	GA	110-94-1	-3.00	-4.03	-2.23		298 K **(SL)**
Pimelic acid	PA	111-16-0	-3.66	-5.10	-3.90		298 K **(SL)**
Tris-(2-ethylhexyl) phosphate	TEHP	78-42-2	-4.52	-6.13	-4.39		298.15 K
Tris-(2-butoxyethyl) phosphate	TBOEP	78-51-3	-4.17	-4.80	-3.76		298.15 K
2,4,4'-Trichlorobiphenyl	PCB-28	7012-37-5	-1.57	-2.05	-1.30		298.15 K **(SL)**
2,2',4,5,5'-Pentachlorobiphenyl	PCB-101	37680-73-2	-2.60	-3.59	-2.52		298.15 K **(SL)**
2,4,5,2‘,4‘,5‘-Hexachlorobiphenyl	PCB-153	35065-27-1	-3.21	-4.61	-3.35		298.15 K **(SL)**
2,2',3,4,4',5,5'-Heptachlorobiphenyl	PCB-180	35065-29-3	-3.96	-5.71	-4.30		298.15 K **(SL)**
1,10-Dichlorodecane	C10Cl2	2162-98-3	-0.30	-0.24	0.42		298.15 K
1,2,11,12-Tetrachlorododecane	C12Cl4	210115-98-3	-2.46	-2.59	-1.77	-2.73 c) 30	298.15 K **(SL)**
2,2′,4,4′-Tetrabromodiphenyl ether	BDE-47	5436-43-1	-3.49	-5.18	-3.90		298.15 K **(SL)**
2,2′,4,4′,5-Pentabromodiphenyl ether	BDE-99	60348-60-9	-4.17	-6.87	-4.92		298.15 K **(SL)**
1,2,3,4,5-Pentabromo-6-ethyl benzene	PBEB	85-22-3	-2.54	-4.23	-3.07	-2.21 31	298.15 K **(SL)**
Dodecamethylcyclohexasiloxane	D6	540-97-6	0.35	-0.23	1.09		298.15 K
Hexadecamethylheptasiloxane	L7	541-01-5	-1.13	-0.27	-0.48		298.15 K
Octadecamethyloctasiloxane	L8	556-69-4	-2.03	-1.08	-1.33		298.15 K
pp‘-DDT	DDT	50-29-3	-3.32	-4.19	-3.77		298.15 K **(SL)**
Diazinon	DZN	333-41-5	-2.23	-3.10	-1.28		298.15 K
Fipronil	FIP	120068-37-3	-5.72	-4.60	-8.35		298.15 K **(SL)**

a) In SPARC it was assumed that the substance is not solid at room temperature

b) Vapor pressure for the subcooled liquid. Calculation: Schwarzenbach et al. (2017), p. 249; data: LFER Database

c) Calculated for all congeners $C_{12}Cl_4$

d) The published reference value for DHP is doubtful.

Table S4: Sampling solvents used for the creation of the CREST ensemble.

Compound	Abbr.	CAS	Sampling solvent
n-Decane	C10	124-18-5	n-Hexadecane
n-Hexadecane	C16	544-76-3	n-Hexadecane
N-Tridecylbenzene	TDB	123-02-4	n-Hexadecane
3-Cresol	3CR	108-39-4	Phenol
Naphthalene	NAP	91-20-3	Benzene
Anthracene	ANT	120-12-7	Benzene
Fluoranthene	FLU	206-44-0	Benzene
2-Butoxy ethanol	EGBE	111-76-2	Diethylether
1-Undecanol	UDC	112-42-5	1-Octanol
Oleyl alcohol	OA	143-28-2	1-Octanol
Glycerol	GLY	56-81-5	Methanol
Benzophenone	BP	119-61-9	Phenol
Benzophenone-3	BP-3	131-57-7	Phenol
Homosalate	HS	118-56-9	Phenol
Dimethyl phthalate	DMP	131-11-3	Phenol
Diethyl phthalate	DEP	84-66-2	Phenol
Di-n-butyl phthalate	DnBP	84-74-2	Phenol
Butyl benzyl phthalate	BBzP	85-68-7	Phenol
Dihexyl phthalate	DHP	84-75-3	Phenol
Di-(2-ethylhexyl) phthalate	DEHP	117-81-7	Phenol
Di-(2-ethylhexyl) terephthalate	DEHTP	6422-86-2	Phenol
Methyl palmitoleate	MP	1120-25-8	Acetone

Glutaric acid	GA	110-94-1	Acetone
Pimelic acid	PA	111-16-0	Acetone
Tris-(2-ethylhexyl) phosphate	TEHP	78-42-2	Acetone
Tris-(2-butoxyethyl) phosphate	TBOEP	78-51-3	Acetone
2,4,4'-Trichlorobiphenyl	PCB-28	7012-37-5	Phenol
2,2',4,5,5'-Pentachlorobiphenyl	PCB-101	37680-73-2	Phenol
2,4,5,2‘,4‘,5‘-Hexachlorobiphenyl	PCB-153	35065-27-1	Dichloromethane
2,2',3,4,4',5,5'-Heptachlorobiphenyl	PCB-180	35065-29-3	Phenol
1,10-Dichlorodecane	C10Cl2	2162-98-3	Dichloromethane
1,2,11,12-Tetrachlorododecane	C12Cl4	210115-98-3	Dichloromethane
2,2′,4,4′-Tetrabromodiphenyl ether	BDE-47	5436-43-1	Dichloromethane
2,2′,4,4′,5-Pentabromodiphenyl ether	BDE-99	60348-60-9	Dichloromethane
1,2,3,4,5-Pentabromo-6-ethyl benzene	PBEB	85-22-3	Dichloromethane
Dodecamethylcyclohexasiloxane	D6	540-97-6	Toluene
Hexadecamethylheptasiloxane	L7	541-01-5	Toluene
Octadecamethyloctasiloxane	L8	556-69-4	Toluene
pp‘-DDT	DDT	50-29-3	Dichloromethane
Diazinon	DZN	333-41-5	Aniline
Fipronil	FIP	120068-37-3	Aniline

Table S5: Log P_L data of the studied compounds with unknown vapor pressure (SL = subcooled liquid). All data for 298 K.

Compounds	Abbr.	CAS	MP (°C)	BP (°C)	log P_L (Pa) (SPARC) [a]	log P_L (Pa) (LFER) [b]	Remark
Plasticizers							
Di-2-propylheptyl phthalate	DPHP	53306-54-0	<25	>400	-8.87	-6.71	
Di-isononyl phthalate [c]	DINP	28553-12-0	-48	>400	-8.04	-6.65	
1,2-Cyclohexane dicarboxylic acid diisononyl ester [d]	DINCH	166412-78-8	<0	394	-6.88	-6.22	
Tri-2-ethylhexyltrimellitate	TOTM	3319-31-1	-46	414	-12.11	-9.15	
Di-iso-butyl adipate	DIBA	141-04-8	-20	279	-1.35	-0.61	
Di-n-butyl adipate	DnBA	105-99-7	-32	305	-1.54	-1.25	
Di-2-ethylhexyl adipate	DEHA	103-23-1	-67	>400	-5.08	-3.92	
Di-isononyl adipate [e]	DINA	33703-08-1	<0	>400	-7.12	-5.16	
Biocides							
Acetamiprid	ACP	135410-20-7	102	352	-2.15	-1.59	SL
Icaridin	ICD	119515-38-7	-	296	-3.08	-2.26	SL
Cyromazine	CMZ	66215-27-8	222	-	-5.19	-4.76	SL
Diflubenzuron	DFB	35367-38-5	232	-	-6.14	-3.66	SL
Cyphenothrin	CPT	39515-40-7	-25	-	-6.96	-7.07	
Methoprene	MTP	40596-69-8	<25	256	-3.54	-1.67	SL
Pharmaceuticals							
Bisoprolol	BPL	66722-44-9	102	445	-6.47	-8.02	SL
Dicloflenac	DIC	15307-86-5	158	-	-6.68	-7.11	SL
Dapagliflozin	DLF	461432-26-8	65	609	-17.85	-19.56	SL
Ibuprofen	IBU	15687-27-1	76	320	-2.3	-2.50	SL
Metoprolol	MPL	51384-51-1	120	399	-4.58	-2.22	SL
Naproxen	NPX	22204-53-1	152	-	-4.65	-5.66	SL
Torasemide	TS	56211-40-6	164	-	-9.66	-13.44	SL

a) It was assumed that the substance is not solid at room temperature

b) Vapor pressure for the subcooled liquid. Calculation: Schwarzenbach et al. (2017), p. 249[32]

c) SMILES is for the isomer bis(7-methyloctyl) phthalate

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

e) SMILES is for the isomer bis(7-methyloctyl) adipate

Table S6: LFER parameters of the reference compounds. All data for 298 K. The data were retrieved from the UFZ-LSER database.[33]

Compound	Abbr.	CAS	L	S	A	B	log P_L (Pa) (LFER)
n-Decane	C10	124-18-5	4.686	0.00	0.00	0.00	2.34
n-Hexadecane	C16	544-76-3	7.771	0.00	0.00	0.00	-0.41
N-Tridecylbenzene	TDB	123-02-4	9.376	0.47	0.00	0.15	-1.93
3-Cresol	3CR	108-39-4	4.310	0.88	0.57	0.34	1.28
Naphthalene	NAP	91-20-3	5.161	0.92	0.00	0.20	1.54
Anthracene	ANT	120-12-7	7.568	1.34	0.00	0.28	-1.02
Fluoranthene	FLU	206-44-0	8.827	1.55	0.00	0.24	-2.40
2-Butoxy ethanol	EGBE	111-76-2	3.806	0.50	0.30	0.83	1.66
1-Undecanol	UDC	112-42-5	6.128	0.42	0.37	0.48	0.01
Oleyl alcohol	OA	143-28-2	9.565	0.58	0.36	0.69	-3.50
Glycerol	GLY	56-81-5	3.145	0.72	0.64	1.21	-0.72
Benzophenone	BP	119-61-9	6.852	1.50	0.00	0.50	-0.58
Benzophenone-3	BP-3	131-57-7	8.840	1.63	0.00	0.62	-2.53
Homosalate	HS	118-56-9	8.614	0.87	0.09	0.48	-1.72
Dimethyl phthalate	DMP	131-11-3	6.050	1.40	0.00	0.86	0.26
Diethyl phthalate	DEP	84-66-2	6.790	1.40	0.00	0.88	-0.40
Di-n-butyl phthalate	DnBP	84-74-2	8.970	1.27	0.00	0.95	-2.18
Butyl benzyl phthalate	BBzP	85-68-7	10.820	1.51	0.00	1.13	-4.12
Dihexyl phthalate	DHP	84-75-3	11.110	1.29	0.00	0.96	-4.11
Di-(2-ethylhexyl) phthalate	DEHP	117-81-7	12.700	1.25	0.00	1.02	-5.48
Di-(2-ethylhexyl) terephthalate	DEHTP	6422-86-2	12.327	1.06	0.00	0.71	-4.96
Methyl palmitoleate	MP	1120-25-8	8.853	0.71	0.00	0.68	-1.59

Glutaric acid	GA	110-94-1	4.207	1.28	1.05	0.75	-2.23
Pimelic acid	PA	111-16-0	5.277	1.26	1.10	0.84	-3.90
Tris-(2-ethylhexyl) phosphate	TEHP	78-42-2	12.091	0.57	0.00	0.88	-4.39
Tris-(2-butoxyethyl)phosphate	TBOEP	78-51-3	10.565	1.40	0.00	2.22	-3.76
2,4,4'-Trichlorobiphenyl	PCB-28	7012-37-5	7.904	1.33	0.00	0.15	-1.30
2,2',4,5,5'-Pentachlorobiphenyl	PCB-101	37680-73-2	8.868	1.61	0.00	0.13	-2.52
2,4,5,2‘,4‘,5‘-Hexachlorobiphenyl	PCB-153	35065-27-1	9.587	1.74	0.00	0.11	-3.35
2,2',3,4,4',5,5'-Heptachlorobiphenyl	PCB-180	35065-29-3	10.415	1.87	0.00	0.09	-4.30
1,10-Dichlorodecane	C10Cl2	2162-98-3	6.466	0.87	0.00	0.17	0.42
1,2,11,12-Tetrachlorododecane	C12Cl4	210115-98-3	8.861	0.94	0.00	0.00	-1.77
2,2′,4,4′-Tetrabromodiphenyl ether	BDE-47	5436-43-1	10.660	1.45	0.00	0.34	-3.90
2,2′,4,4′,5-Pentabromodiphenyl ether	BDE-99	60348-60-9	11.710	1.51	0.00	0.44	-4.92
1,2,3,4,5-Pentabromo-6-ethyl benzene	PBEB	85-22-3	9.848	1.36	0.00	0.00	-3.07
Dodecamethylcyclohexasiloxane	D6	540-97-6	6.080	-0.12	0.00	0.74	1.09
Hexadecamethylheptasiloxane	L7	541-01-5	7.838	-0.20	0.00	0.94	-0.48
Octadecamethyloctasiloxane	L8	556-69-4	8.787	-0.23	0.00	1.08	-1.33
pp‘-DDT	DDT	50-29-3	10.020	1.76	0.00	0.16	-3.77
Diazinon	DZN	333-41-5	8.001	0.81	0.06	1.18	-1.28
Fipronil	FIP	120068-37-3	10.065	2.81	0.29	1.54	-8.35

Table S7: LFER parameters of the studied compounds with unknown vapor pressure. All data for 298 K. The data were retrieved from the UFZ-LSER database.[33]

Compound	Abbr.	CAS	L	S	A	B	log P_L (Pa) (LFER) [a]
Plasticizers							
Di-2-propylheptyl phthalate	DPHP	53306-54-0	14.30	1.06	0.00	0.90	-6.71
Di-isononyl phthalate [b]	DINP	28553-12-0	13.99	1.27	0.00	1.02	-6.65
1,2-Cyclohexane dicarboxylic acid diisononyl ester [c]	DINCH	166412-78-8	13.682	1.12	0.00	0.99	-6.22
Tri-2-ethylhexyltrimellitate	TOTM	3319-31-1	17.017	1.08	0.00	1.02	-9.15
Di-iso-butyl adipate	DIBA	141-04-8	7.586	0.92	0.00	0.97	-0.61
Di-n-butyl adipate	DnBA	105-99-7	8.102	1.12	0.00	1.03	-1.25
Di-2-ethylhexyl adipate	DEHA	103-23-1	11.297	0.92	0.00	0.97	-3.92
Di-isononyl adipate [d]	DINA	33703-08-1	12.478	1.13	0.00	1.10	-5.16
Biocides							
Acetamiprid	ACP	135410-20-7	7.51	1.57	0.05	1.21	-1.59
Icaridin	ICD	119515-38-7	7.397	1.03	0.33	0.96	-2.26
Cyromazine	CMZ	66215-27-8	6.929	1.74	0.56	1.24	-4.76
Diflubenzuron	DFB	35367-38-5	9.68	1.17	0.18	0.97	-3.66
Cyphenothrin	CPT	39515-40-7	12.326	2.29	0.05	1.11	-7.07
Methoprene	MTP	40596-69-8	8.976	0.66	0.00	0.97	-1.67
Pharmaceuticals							
Bisoprolol	BPL	66722-44-9	11.2	1.50	0.30	2.19	-8.02
Dicloflenac	DIC	15307-86-5	11.025	1.85	0.55	0.77	-7.11
Dapagliflozin	DLF	461432-26-8	14.465	2.58	0.97	1.95	-19.56
Ibuprofen	IBU	15687-27-1	7.184	0.70	0.56	0.79	-2.50
Metoprolol	MPL	51384-51-1	9.157	1.61	-0.06	1.72	-2.22
Naproxen	NPX	22204-53-1	9.207	2.02	0.60	0.67	-5.66
Torasemid	TS	56211-40-6	13.23	2.18	0.70	1.60	-13.44

a) Vapor pressure for the subcooled liquid. Calculation: Schwarzenbach et al. (2017), p. 249[32]

b) SMILES is for the isomer bis(7-methyloctyl) phthalate

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

d) SMILES is for the isomer bis(7-methyloctyl) adipate

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