Supplementary material

Structure-activity relationships to estimate the effective Henry's law coefficients of organics of atmospheric interest

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– Table S1 : Effective Henry's constants collected from literature and predicted using GROMHE, SPARC and HWIN$_b$.

– Table S2 : Hydration constants from literature and estimated using our SAR for aldehydes and ketones in log units.

– References.

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Table S1 : Effective Henry's constants collected from literature and predicted using GROMHE, SPARC and $HWIN_b$.

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
Hydrocarbon							
CC	74-84-0	T	-2.7	-2.7	-2.9	-2.7	Sander (1999)
CCC	74-98-6	T	-2.8	-2.8	-2.9	-2.9	Sander (1999)
CCCC	106-97-8	T	-3.0	-2.9	-2.8	-3.0	Mackay and Shiu (1981)
CC(C)(C)C	463-82-1	T	-3.6	-3.1	-3.6	-3.1	Mackay and Shiu (1981)
CC(C)C	75-28-5	T	-3.1	-2.9	-3.2	-3.0	Mackay and Shiu (1981)
CCC(C)C	78-78-4	V	-3.1	-3.1	-3.1	-3.1	Mackay and Shiu (1981)
CCCCC	109-66-0	T	-3.1	-3.1	-2.9	-3.1	Mackay and Shiu (1981)
CCCC(C)C	107-83-5	T	-3.2	-3.2	-3.2	-3.2	Mackay and Shiu (1981)
CCC(C)CC	96-14-0	V	-3.2	-3.2	-3.1	-3.2	Mackay and Shiu (1981)
CCC(C)(C)C	75-83-2	V	-3.2	-3.2	-3.5	-3.2	Mackay and Shiu (1981)
CC(C)C(C)C	79-29-8	T	-3.1	-3.2	-3.2	-3.2	Mackay and Shiu (1981)
CCCC(C)(C)C	590-35-2	T	-3.5	-3.3	-3.6	-3.4	Mackay and Shiu (1981)
CCC(C)C(C)C	565-59-3	T	-3.2	-3.3	-3.3	-3.4	Mackay and Shiu (1981)
CC(C)CC(C)C	108-08-7	T	-3.5	-3.3	-3.6	-3.4	Mackay and Shiu (1981)
CCCCCCCC	111-65-9	T	-3.5	-3.4	-3.3	-3.5	Mackay and Shiu (1981)
CCCCC(C)CC	589-81-1	T	-3.6	-3.4	-3.4	-3.5	Mackay and Shiu (1981)
CC(C)CC(C)(C)C	540-84-1	T	-3.5	-3.4	-3.9	-3.5	Mackay and Shiu (1981)
CC(C)C(C)C(C)C	565-75-3	T	-3.3	-3.4	-3.5	-3.5	Mackay and Shiu (1981)
CCCCCCCCC	111-84-2	V	-3.7	-3.6	-3.4	-3.6	Mackay and Shiu (1981)
CCCCC(C)CCC	2216-34-4	T	-4.0	-3.6	-3.5	-3.6	Mackay and Shiu (1981)
CCCCCCCCCC	124-18-5	T	-3.9	-3.7	-3.5	-3.7	Mackay and Shiu (1981)
CCCCCCCCCCCC	112-40-3	T	-3.9	-3.9	-3.8	-4.0	Mackay and Shiu (1981)
CCCCCCC	142-82-5	V	-2.9	-3.3	-3.1	-3.4	Sander (1999)
CCCCCC	110-54-3	T	-3.2	-3.2	-3.0	-3.2	Mackay and Shiu (1981)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
CCCCC(C)C	591-76-4	V	-2.7	-3.3	-3.4	-3.4	Sander (1999)
C1CC1	75-19-4	V	-1.9	-2.2	-1.8	-2.0	Wilhelm et al. (1977)
C1CCCC1	287-92-3	T	-2.2	-2.4	-1.9	-2.3	Sander (1999)
C1CCCC1C	96-37-7	V	-2.6	-2.6	-2.3	-2.4	Mackay and Shiu (1981)
C1CCCCC1C	108-87-2	V	-2.0	-2.7	-2.4	-2.5	Sander (1999)
CC1CCCCC1C	583-57-3	V	-2.6	-2.8	-2.8	-2.7	Mackay and Shiu (1981)
C1CC(C)CCC1C	2207-04-7	T	-3.0	-2.8	-2.8	-2.7	Mackay and Shiu (1981)
C1C(C)CCC1(C)C	4516-69-2	V	-3.2	-2.8	-3.2	-2.7	Mackay and Shiu (1981)
C1CCCC1CCC	2040-96-2	T	-3.0	-2.8	-2.6	-2.7	Mackay and Shiu (1981)
C1CCCC1CCCCC	3741-00-2	T	-3.3	-3.1	-2.9	-2.9	Mackay and Shiu (1981)
C1CCCCCC1	291-64-5	T	-2.0	-2.7	-2.2	-2.5	Meylan and Howard (2000)
C1CCCCC1CC	1678-91-7	T	-2.5	-2.8	-2.5	-2.7	Meylan and Howard (2000)
C=C	74-85-1	T	-2.3	-2.1	-2.6	-2.0	Wilhelm et al. (1977)
CC=C	115-07-1	T	-2.3	-2.2	-2.0	-2.2	Mackay and Shiu (1981)
CCC=C	106-98-9	T	-2.9	-2.3	-2.2	-2.3	Mackay and Shiu (1981)
CC(C)=C	115-11-7	T	-2.8	-2.3	-2.0	-2.4	Mackay and Shiu (1981)
CCCC=C	109-67-1	V	-2.6	-2.4	-2.5	-2.4	Mackay and Shiu (1981)
CC(C)C=C	563-45-1	T	-2.7	-2.4	-2.7	-2.4	Mackay and Shiu (1981)
CCCCC=C	592-41-6	T	-2.6	-2.6	-2.7	-2.6	Mackay and Shiu (1981)
CCCC(C)=C	763-29-1	V	-2.4	-2.6	-2.5	-2.6	Mackay and Shiu (1981)
CC(C)CC=C	691-37-2	T	-2.8	-2.6	-2.8	-2.6	Mackay and Shiu (1981)
CCCCC=CC	592-77-8	V	-2.6	-2.7	-2.7	-2.8	Mackay and Shiu (1981)
CCCCCCC=C	111-66-0	T	-3.0	-2.8	-3.0	-2.8	Mackay and Shiu (1981)
C=CC=C	106-99-0	T	-1.9	-1.7	-2.0	-1.9	Wilhelm et al. (1977)
C=CC(C)=C	78-79-5	T	-1.6	-1.8	-1.8	-2.1	Sander (1999)
C=CCC=C	591-93-5	T	-2.1	-1.8	-2.1	-2.1	Mackay and Shiu (1981)
C1CC=CCC1	110-83-8	T	-1.6	-2.0	-1.6	-1.8	Nielsen et al. (1994)
C1C=CCC=C1	628-41-1	V	-1.0	-1.3	-1.2	-2.0	Meylan and Howard (2000)
C1CC=CC1	142-29-0	T	-1.8	-1.8	-1.5	-1.7	Meylan and Howard (2000)
CC(C)=CCCC(=C)C=C	123-35-3	V	-1.8	-1.8	-2.2	-2.7	Meylan and Howard (2000)
C1CC=CCC1C=C	100-40-3	V	-1.7	-1.6	-1.8	-2.2	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
c1ccccc1	71-43-2	T	-0.7	-0.7	-0.8	-0.7	Dewulf et al. (1995)
c1ccccc1CC	100-41-4	T	-0.8	-1.0	-1.0	-0.9	Robbins et al. (1993)
c1c(C)cccc1C	108-38-3	T	-0.8	-1.0	-0.9	-0.8	Dewulf et al. (1995)
c1ccccc1C	108-88-3	T	-0.7	-0.8	-0.9	-0.8	Dewulf et al. (1995)
CCc1ccccc1CC	135-01-3	V	-0.4	-1.2	-1.0	-1.1	Meylan and Howard (2000)
Cc1ccccc1C	95-47-6	T	-0.6	-1.0	-0.8	-0.8	Dewulf et al. (1995)
c1cc(C)ccc1C	106-42-3	V	-0.8	-1.0	-0.8	-0.8	Dewulf et al. (1995)
Cc1ccc(C)cc1C	95-63-6	T	-0.8	-1.1	-0.7	-0.9	Sander (1999)
c1ccccc1CCC	103-65-1	T	-0.9	-1.1	-1.1	-1.0	Mackay and Shiu (1981)
c1ccccc1C(C)C	98-82-8	T	-0.1	-1.1	-1.2	-1.0	Mackay and Shiu (1981)
Cc1ccccc1CC	611-14-3	V	-0.6	-1.1	-0.8	-0.9	Mackay and Shiu (1981)
CCc1ccccc1CCC	16021-20-8	T	-1.5	-1.2	-1.2	-1.2	Mackay and Shiu (1981)
c1ccccc1C(C)(C)CC	2049-95-8	T	-1.1	-1.3	-1.2	-1.3	Mackay and Shiu (1981)
c1cc(C)ccc1C(C)C	99-87-6	V	-0.9	-1.2	-1.1	-1.1	Mackay and Shiu (1981)
c1ccccc1CCCCC	538-68-1	V	-0.8	-1.3	-1.4	-1.3	Mackay and Shiu (1981)
c1ccccc1C=C	100-42-5	T	-0.4	-0.3	-0.6	-0.4	Meylan and Howard (2000)
c1ccccc1CCCC	104-51-8	V	-1.2	-1.2	-1.3	-1.1	Meylan and Howard (2000)
c1ccccc1C(C)CC	135-98-8	T	-1.2	-1.2	-1.1	-1.1	Meylan and Howard (2000)
Cc1cccc(C)c1C	526-73-8	T	-0.6	-1.1	-0.6	-0.9	Meylan and Howard (2000)
Cc1ccccc1C(C)C	527-84-4	V	-1.1	-1.2	-1.0	-1.1	Meylan and Howard (2000)
c1cc(C)ccc1C=C	622-97-9	T	-0.5	-0.5	-0.6	-0.5	Meylan and Howard (2000)
Monofunctional							
CC=CC(O)	6117-91-5	T	2.5	2.5	2.6	2.1	Hilal et al. (2008)
CC(O)(C)C=C	115-18-4	T	1.8	2.4	1.8	2.0	Hilal et al. (2008)
C(O)	67-56-1	T	2.3	2.3	2.0	2.4	Sander (1999)
CC(O)	64-17-5	T	2.3	2.2	2.2	2.2	Sander (1999)
CCC(O)	71-23-8	T	2.1	2.1	1.9	2.1	Sander (1999)
CC(O)C	67-63-0	T	2.1	2.1	1.8	2.1	Sander (1999)
CCCC(O)	71-36-3	T	2.1	1.9	1.8	2.0	Sander (1999)

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				GROMHE	*SPARC*	$HWIN_b$	
CC(C)C(O)	78-83-1	T	2.0	1.9	1.8	2.0	Sander (1999)
CCC(O)C	78-92-2	T	2.0	1.9	1.7	2.0	Sander (1999)
CC(O)(C)C	75-65-0	T	1.8	1.9	1.5	2.0	Sander (1999)
CCC(O)(C)C	75-85-4	V	1.9	1.8	1.6	1.9	Butler and Ramchandani (1935)
CCCCC(O)	71-41-0	T	1.9	1.8	1.6	1.9	Butler and Ramchandani (1935)
CCCC(O)C	6032-29-7	V	1.8	1.8	1.6	1.9	Butler and Ramchandani (1935)
CCCCCC(O)	111-27-3	V	1.8	1.7	1.5	1.8	Buttery et al. (1969)
CCC(C)C(O)	137-32-6	T	1.9	1.8	1.7	1.9	Butler and Ramchandani (1935)
CCCCCCCC(O)	111-87-5	T	1.6	1.4	1.3	1.5	Buttery et al. (1969)
CCC(O)CC	584-02-1	T	1.7	1.8	1.6	1.9	Meylan and Howard (2000)
CC(O)C(C)C	598-75-4	V	1.8	1.8	1.6	1.9	Meylan and Howard (2000)
CCCCC(O)C	626-93-7	V	1.6	1.7	1.4	1.8	Meylan and Howard (2000)
CCCC(O)CC	623-37-0	T	1.4	1.7	1.5	1.8	Meylan and Howard (2000)
CCCC(C)C(O)	105-30-6	V	1.4	1.7	1.6	1.8	Meylan and Howard (2000)
CCCC(O)(C)C	590-36-3	T	1.4	1.7	1.5	1.8	Meylan and Howard (2000)
CC(C)CC(O)	123-51-3	V	1.9	1.8	1.7	1.9	Butler and Ramchandani (1935)
CC(O)CC(C)C	108-11-2	T	1.3	1.7	1.5	1.8	Hine and Mookerjee (1975)
CCC(C(O))CC	97-95-0	T	1.3	1.7	1.6	1.8	Meylan and Howard (2000)
CCCCCCC(O)	111-70-6	V	1.7	1.6	1.4	1.6	Butler and Ramchandani (1935)
CCCCCC(O)C	543-49-7	T	1.3	1.6	1.3	1.6	Meylan and Howard (2000)
CCCCC(O)CC	589-82-2	T	1.5	1.6	1.4	1.6	Meylan and Howard (2000)
CCCCCCC(O)C	123-96-6	V	0.9	1.4	1.2	1.5	Meylan and Howard (2000)
CCCCC(C(O))CC	104-76-7	V	1.6	1.4	1.5	1.5	Meylan and Howard (2000)
CCCCCCCCC(O)	143-08-8	V	1.5	1.3	1.2	1.4	Meylan and Howard (2000)
CCCCCCCC(O)C	628-99-9	T	1.3	1.3	1.1	1.4	Meylan and Howard (2000)
CC(C)CC(O)CC(C)C	108-82-7	T	0.9	1.3	1.2	1.4	Meylan and Howard (2000)
CCCCCCCCCC(O)	112-30-1	V	1.5	1.2	1.1	1.3	Altschuh et al. (1999)
CCCCCCCCCCCC(O)	112-53-8	T	1.7	0.9	1.0	1.0	Altschuh et al. (1999)
CC(C)(C)C(O)	75-84-3	T	1.3	1.8	1.6	1.9	Meylan and Howard (2000)
CCC(O)(C)CC	77-74-7	T	1.8	1.7	1.5	1.8	Meylan and Howard (2000)
C(O)C=C	107-18-6	T	2.3	2.7	2.6	2.2	Hine and Mookerjee (1975)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
C1CCC(O)CC1	108-93-0	T	2.4	2.3	2.4	2.3	Altschuh et al. (1999)
C1CCCC(O)C1C	583-59-5	T	2.1	2.2	2.2	2.2	Altschuh et al. (1999)
C1CCC(O)CC1C	591-23-1	T	2.4	2.2	2.2	2.2	Altschuh et al. (1999)
c1ccccc1CC(O)	60-12-8	T	3.6	3.9	3.4	3.5	Abraham et al. (1994)
c1ccccc1C(O)	100-51-6	T	3.5	4.0	3.6	3.7	Abraham et al. (1994)
Cc1ccc(O)cc1C	95-65-8	T	3.4	2.8	2.9	3.2	Abraham et al. (1994)
c1cc(C)c(O)cc1C	95-87-4	T	2.9	2.8	2.8	3.2	Abraham et al. (1994)
c1cccc(O)c1CC	90-00-6	T	2.3	2.8	2.7	3.1	Meylan and Howard (2000)
c1c(C)c(O)ccc1C	105-67-9	T	3.0	2.8	2.8	3.2	Abraham et al. (1994)
c1c(C)cc(O)cc1C	108-68-9	T	3.2	2.8	2.7	3.2	Abraham et al. (1994)
c1cc(O)ccc1CC	123-07-9	V	3.1	2.8	2.8	3.1	Abraham et al. (1994)
Cc1cccc(O)c1C	526-75-0	T	3.1	2.8	2.9	3.2	Abraham et al. (1994)
c1c(C)c(O)c(C)cc1C	527-60-6	T	2.6	2.7	2.5	3.1	Meylan and Howard (2000)
c1ccc(C)c(O)c1C	576-26-1	T	2.2	2.8	2.6	3.2	Hawthorne et al. (1985)
c1cc(O)ccc1CCC	645-56-7	V	2.9	2.7	2.6	3.0	Abraham et al. (1994)
c1c(C)cc(O)cc1CC	698-71-5	T	3.2	2.7	2.6	3.0	Meylan and Howard (2000)
c1cc(C)cc(O)c1C(C)C	89-83-8	T	3.3	2.5	2.3	2.9	Meylan and Howard (2000)
c1ccc(O)cc1CC	620-17-7	T	3.2	2.8	2.7	3.1	Abraham et al. (1994)
c1ccc(O)cc1	108-95-2	T	3.5	3.0	2.9	3.2	Gaffney et al. (1987b)
C(OO)	3031-73-0	V	2.5	2.7	2.1	2.2	O'Sullivan et al. (1996)
CC(OO)	3031-74-1	V	2.5	2.6	2.0	2.0	O'Sullivan et al. (1996)
CC(C)-O-C(C)C	108-20-3	T	-0.3	-0.4	-0.2	-0.4	Nielsen et al. (1994)
CCC-O-CCC	111-43-3	T	-0.6	-0.4	-0.1	-0.4	Hartkopf and Karger (1973)
CC-O-CC	60-29-7	T	0.1	-0.2	0.1	-0.2	Nielsen et al. (1994)
C-O-C(C)(C)C	1634-04-4	T	0.2	-0.3	-0.2	-0.3	Robbins et al. (1993)
CC-O-C=C	109-92-2	T	-0.7	-0.2	-1.4	-0.9	Meylan and Howard (2000)
C=C-O-C=C	109-93-3	T	-0.9	-0.1	-1.4	-1.6	Meylan and Howard (2000)
CCCC-O-C=C	111-34-2	T	-0.3	-0.4	-1.7	-1.1	Meylan and Howard (2000)
CCCC-O-CCCC	142-96-1	T	-0.8	-0.7	-0.2	-0.7	Hine and Moorkerjee (1975)
CC(C)CC-O-CCC(C)C	544-01-4	T	-0.2	-0.9	-0.3	-0.9	Meylan and Howard (2000)
CCC-O-C	557-17-5	V	-0.2	-0.2	0.2	-0.2	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
C-O-C(C)C	598-53-8	T	0.0	-0.2	0.1	-0.2	Meylan and Howard (2000)
CCC-O-C(C)C	627-08-7	T	-0.4	-0.4	-0.2	-0.4	Meylan and Howard (2000)
CCCC-O-C	628-28-4	T	-0.3	-0.3	0.1	-0.3	Meylan and Howard (2000)
CCC-O-CC	628-32-0	T	-0.1	-0.3	0.0	-0.3	Meylan and Howard (2000)
CC-O-C(C)(C)CC	919-94-8	T	-1.3	-0.6	-0.5	-0.6	Meylan and Howard (2000)
CCC(C)-O-C	6795-87-5	T	-0.2	-0.3	0.0	-0.3	Meylan and Howard (2000)
c1ccccc1-O-CC	103-73-1	T	0.4	0.7	-0.1	0.4	Meylan and Howard (2000)
CC(=O)	75-07-0	T	1.1	1.2	1.6	1.2	Staudinger and Roberts (1996)
CCC(=O)	123-38-6	T	1.1	1.1	1.4	1.0	Zhou and Mopper (1990)
CCCC(=O)	123-72-8	T	1.0	1.0	1.1	0.9	Zhou and Mopper (1990)
CCCCC(=O)	110-62-3	T	0.8	0.8	0.9	0.8	Zhou and Mopper (1990)
CCCCCC(=O)	66-25-1	T	0.7	0.7	0.7	0.7	Zhou and Mopper (1990)
CCCCCCC(=O)	111-71-7	T	0.5	0.6	0.6	0.6	Zhou and Mopper (1990)
CCCCCCCC(=O)	124-13-0	T	0.3	0.5	0.5	0.4	Zhou and Mopper (1990)
CCCCCCCCC(=O)	124-19-6	T	0.0	0.3	0.6	0.3	Zhou and Mopper (1990)
CCCCCCCCCC(=O)	112-31-2	V	-0.2	0.2	1.0	0.2	Zhou and Mopper (1990)
C(=O)C=C	107-02-8	T	0.9	0.8	1.1	1.5	Snider and Dawson (1985)
CC(C(=O))=C	78-85-3	T	0.8	0.6	1.0	1.2	Iraci et al. (1999)
CC(=O)C	67-64-1	V	1.5	1.4	1.3	1.3	Staudingers and Roberts (1996)
CCC(=O)C	78-93-3	T	1.3	1.3	1.2	1.2	Staudingers and Roberts (1996)
CCCC(=O)C	107-87-9	T	1.2	1.2	0.9	1.1	Buttery et al. (1971)
CCCCCC(=O)C	110-43-0	V	0.8	0.9	0.6	0.8	Buttery et al. (1971)
CCCCCCC(=O)C	111-13-7	V	0.7	0.8	0.6	0.7	Buttery et al. (1971)
CCCCCCCC(=O)C	821-55-6	T	0.4	0.7	0.6	0.6	Buttery et al. (1971)
CCCCCCCCCC(=O)C	112-12-9	T	0.2	0.4	1.7	0.3	Buttery et al. (1971)
CC(=O)C=C	78-94-4	V	1.6	1.3	1.3	1.6	Meylan and Howard (2000)
CC(=O)C(C)(C)C	75-97-8	T	0.7	1.0	0.5	0.9	Meylan and Howard (2000)
C1C(C)=CC(=O)CC1(C)C	78-59-1	T	2.2	1.3	2.0	1.2	Meylan and Howard (2000)
C1CCC(=O)CC1	108-94-1	T	2.0	1.6	2.0	1.3	Meylan and Howard (2000)
C1CC(=O)CC1	120-92-3	T	2.0	1.8	2.0	1.4	Meylan and Howard (2000)
CCC(=O)CC	96-22-0	T	1.0	1.2	0.9	1.1	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
CCCCC(C=O)CC	123-05-7	T	0.1	0.5	0.3	0.4	Meylan and Howard (2000)
CCCC(=O)CCC	123-19-3	T	1.3	0.9	0.5	0.8	Meylan and Howard (2000)
CC(=O)C=C(C)C	141-79-7	V	1.4	1.0	1.2	1.2	Meylan and Howard (2000)
CC(=O)C(C)C	563-80-4	V	1.0	1.2	0.8	1.1	Meylan and Howard (2000)
CCC(C)C(=O)C	565-61-7	T	1.1	1.0	0.8	0.9	Meylan and Howard (2000)
CCC(=O)C(C)C	565-69-5	T	0.8	1.0	0.7	0.9	Meylan and Howard (2000)
CC(C)C(=O)C(C)C	565-80-0	V	0.5	0.9	0.4	0.8	Meylan and Howard (2000)
c1ccccc1C(=O)	100-52-7	V	1.6	1.6	1.7	1.9	Zhou and Mopper (1990)
c1ccccc1C(=O)C	98-86-2	T	2.0	2.1	2.0	2.0	Betterton (1991)
CC(=O)O	64-19-7	T	3.6	3.3	4.1	3.3	Johnson et al. (1996)
CCC(=O)(O)	79-09-4	T	3.8	3.2	4.1	3.1	Khan et al. (1995)
CCCC(=O)(O)	107-92-6	V	3.7	3.1	3.8	3.0	Khan et al. (1995)
CC(C)C(=O)(O)	79-31-2	T	3.0	3.1	3.5	3.0	Khan et al. (1995)
CCCCC(=O)(O)	109-52-4	T	3.3	3.0	3.5	2.9	Khan et al. (1995)
CCCCCC(=O)(O)	142-62-1	T	3.1	2.8	3.4	2.8	Khan et al. (1995)
CC(C)CC(=O)(O)	503-74-2	T	3.1	3.0	3.6	2.9	Khan et al. (1995)
CC(C)(C)C(=O)(O)	75-98-9	T	2.5	3.0	3.0	2.9	Khan et al. (1995)
CC(C(=O)(O))=C	79-41-4	T	3.4	3.1	3.0	3.3	Khan et al. (1995)
C(=O)(O)C=C	79-10-7	T	3.4	3.2	3.0	3.5	Meylan and Howard (2000)
CCC(C(=O)(O))CC	88-09-5	T	2.8	2.8	3.0	2.8	Meylan and Howard (2000)
CC=CC(=O)(O)	503-64-0	T	4.2	3.1	3.1	3.3	Meylan and Howard (2000)
c1ccccc1C=CC(=O)(O)	621-82-9	T	4.8	5.0	4.2	4.9	Meylan and Howard (2000)
c1ccccc1C(=O)(O)	65-85-0	T	4.4	4.1	4.2	4.0	Meylan and Howard (2000)
c1ccccc1CC(=O)(O)	103-82-2	T	4.4	5.1	5.1	4.3	Meylan and Howard (2000)
CC(=O)(OO)	79-21-0	T	2.9	2.9	2.4	2.9	O'Sullivan et al. (1996)
C-O-C(=O)C(C)=C	80-62-6	V	0.5	0.7	0.7	0.8	Hilal et al. (2008)
CC-O-C(=O)C(C)=C	97-63-2	T	0.2	0.5	0.5	0.7	Hilal et al. (2008)
CC(C)C-O-C(=O)C(C)=C	97-86-9	V	0.3	0.3	0.3	0.5	Hilal et al. (2008)
CC(=O)-O-C=C	108-05-4	T	0.2	0.8	0.9	-0.1	Hilal et al. (2008)
CC(=O)-O-C	79-20-9	V	0.9	0.9	0.9	0.8	Kieckbusch and King (1979)
CC-O-C(=O)C	141-78-6	T	0.8	0.8	0.6	0.6	Kieckbusch and King (1979)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
CCC(=O)-O-C	554-12-1	T	0.8	0.8	0.6	0.6	Buttery et al. (1969)
CCC-O-C(=O)C	109-60-4	T	0.7	0.6	0.5	0.5	Kieckbusch and King (1979)
CCCC(=O)-O-C	623-42-7	T	0.7	0.6	0.4	0.5	Buttery et al. (1969)
CCCC-O-C(=O)C	123-86-4	T	0.6	0.5	0.3	0.4	Kieckbusch and King (1979)
C-O-C(=O)	107-31-3	T	0.6	0.6	0.9	0.6	Hartkopf et al. (1973)
CCCCC(=O)-O-C	624-24-8	V	0.5	0.5	0.3	0.4	Buttery et al. (1969)
CCCCCC(=O)-O-C	106-70-7	T	0.4	0.4	0.2	0.3	Buttery et al. (1969)
CCCCCCCC(=O)-O-C	111-11-5	T	0.1	0.1	0.1	0.0	Buttery et al. (1969)
CCC-O-C(=O)	110-74-7	T	0.4	0.4	0.3	0.4	Meylan and Howard (2000)
CCCC-O-C(=O)	592-84-7	T	0.3	0.3	0.2	0.2	Meylan and Howard (2000)
CC-O-C(=O)	109-94-4	V	0.4	0.5	0.6	0.5	Hartkopf et al. (1973)
C-O-C(=O)C=C	96-33-3	T	0.7	0.8	0.8	1.0	Meylan and Howard (2000)
CCC(=O)-O-CC	105-37-3	V	0.6	0.6	0.4	0.5	Meylan and Howard (2000)
CCCC(=O)-O-CCC	105-66-8	T	0.2	0.4	0.1	0.3	Meylan and Howard (2000)
CCCCCCC(=O)-O-CC	106-30-9	V	0.3	0.1	-0.1	0.0	Meylan and Howard (2000)
CC(C)C-O-C(=O)C(C)C	97-85-8	T	0.1	0.3	0.1	0.1	Meylan and Howard (2000)
CCCC-O-C(=O)C(C)=C	97-88-1	T	0.3	0.3	0.2	0.5	Meylan and Howard (2000)
CCCC-O-C(=O)CCC	109-21-7	T	0.2	0.3	0.0	0.1	Meylan and Howard (2000)
CCC-O-C(=O)CC	106-36-5	V	0.4	0.5	0.3	0.4	Meylan and Howard (2000)
CC(C)C-O-C(=O)C=C	106-63-8	T	0.1	0.4	0.4	0.7	Meylan and Howard (2000)
CC-O-C(=O)CC(C)C	108-64-5	V	0.1	0.4	0.2	0.3	Meylan and Howard (2000)
CC(=O)-O-CCC(C)C	123-92-2	V	0.2	0.4	0.4	0.3	Meylan and Howard (2000)
CC-O-C(=O)C=C	140-88-5	T	0.5	0.7	0.6	0.9	Meylan and Howard (2000)
CCCC-O-C(=O)C=C	141-32-2	T	0.3	0.4	0.3	0.7	Meylan and Howard (2000)
CCCCC(=O)-O-CC	539-82-2	T	0.4	0.4	0.2	0.3	Meylan and Howard (2000)
C-O-C(=O)C(C)(C)C	598-98-1	T	0.4	0.5	0.2	0.4	Meylan and Howard (2000)
CCCCC-O-C(=O)CC	624-54-4	T	0.1	0.3	0.1	0.1	Meylan and Howard (2000)
CCCCC-O-C(=O)C	628-63-7	V	0.4	0.4	0.3	0.3	Meylan and Howard (2000)
CCCCC(CC)C-O-C(=O)C=C	103-11-7	V	0.4	-0.1	0.1	0.2	Meylan and Howard (2000)
c1ccccc1C(=O)-O-CCCC	136-60-7	T	1.4	1.3	1.0	1.1	Meylan and Howard (2000)
c1ccccc1C(=O)-O-CC	93-89-0	T	1.1	1.5	1.3	1.3	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
CO(N(=O)=O)	598-58-3	T	0.3	0.1	0.8	0.7	Kames and Schurath (1992)
CCO(N(=O)=O)	625-58-1	T	0.2	0.0	0.6	0.6	Kames and Schurath (1992)
CCCO(N(=O)=O)	627-13-4	T	-0.1	-0.1	0.3	0.5	Hauff et al. (1998)
CCO(N(=O)=O)C	1712-64-7	T	-0.2	-0.1	0.2	2.7	Hauff et al. (1998)
CCCC(ON(=O)=O)	928-45-0	T	-0.2	-0.3	0.1	0.3	Hauff et al. (1998)
CCC(ON(=O)=O)C	543-29-3	V	-0.4	-0.3	0.0	0.3	Hauff et al. (1998)
CC(ON(=O)=O)(C)C	*n.a.*	T	-0.2	-0.3	-0.2	0.3	Kames and Schurath (1992)
CCCCC(ON(=O)=O)	1002-16-0	V	-0.2	-0.4	0.0	0.2	Hauff et al. (1998)
CCCCO(N(=O)=O)C	928-45-0	T	-0.5	-0.4	-0.2	2.4	Hauff et al. (1998)
CC(C)CC(ON(=O)=O)	543-87-3	V	-0.3	-0.4	0.0	0.2	Hauff et al. (1998)
CCCCCC(ON(=O)=O)	633-11-8	V	-0.2	-0.5	-0.2	0.1	Hauff et al. (1998)
CCC(ON(=O)=O)CC	8294-459-0	T	-0.4	-0.4	-0.2	0.2	Hauff et al. (1998)
C(N(=O)=O)	75-52-5	T	1.7	1.1	1.3	1.4	Rohrschn. (1973)
CC(N(=O)=O)	79-24-3	T	1.3	1.0	1.3	1.2	Meylan and Howard (2000)
CC(N(=O)=O)C	79-46-9	T	0.9	0.9	0.8	1.1	Meylan and Howard (2000)
CCC(N(=O)=O)	108-03-2	T	1.0	0.9	1.0	1.1	Hine and Moorkerjee (1975)
c1cccc(N(=O)=O)c1C	88-72-2	T	1.9	1.7	1.4	1.6	Meylan and Howard (2000)
CC(=O)(OON(=O)=O)	2278-22-0	V	0.6	0.5	2.7	0.9	Kames and Schurath (1995)
CCC(=O)(OON(=O)=O)	5796-89-4	T	0.5	0.4	2.3	0.8	Kames and Schurath (1995)
CCCC(=O)(OON(=O)=O)	*n.a.*	T	0.4	0.2	2.1	0.7	Kames and Schurath (1995)
C(C=C)(=O)(OON(=O)=O)	*n.a.*	V	0.2	0.3	2.5	1.2	Kames and Schurath (1995)
CC(C)C(=O)(OON(=O)=O)	*n.a.*	T	0.0	0.2	2.1	0.7	Kames and Schurath (1995)
CC(C)=CCCC(O)(C)C=C	78-70-6	V	1.7	2.4	1.8	1.4	Hilal et al. (2008)
C(F)	593-53-3	T	-1.3	-1.3	-1.2	-1.2	Mackay and Shiu (1981)
CC(F)	353-36-6	V	-1.3	-1.5	-1.2	-1.3	Meylan and Howard (2000)
c1ccc(F)cc1	462-06-6	T	-0.8	-0.6	-0.8	-0.8	Mackay and Shiu (1981)
C(Cl)	74-87-3	V	-0.9	-1.1	-0.9	-0.9	Gossett (1987)
CC(Cl)	75-00-3	V	-1.1	-1.2	-0.9	-1.0	Staudinger and Roberts (1996)
CCC(Cl)	540-54-5	V	-1.1	-1.3	-1.1	-1.2	Gossett (1987)
CC(C)C(Cl)	513-36-0	T	-1.3	-1.4	-1.2	-1.3	Meylan and Howard (2000)
C(Cl)=C	75-01-4	V	-1.4	-1.2	-1.6	-1.6	Staudinger and Roberts (1996)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
CCCC(Cl)	109-69-3	T	-1.3	-1.4	-1.2	-1.3	Meylan and Howard (2000)
CC(Cl)(C)C	507-20-0	V	-1.1	-1.4	-1.6	-1.3	Meylan and Howard (2000)
CC(Cl)C	75-29-6	V	-1.2	-1.3	-1.3	-1.2	Meylan and Howard (2000)
CCC(Cl)C	78-86-4	T	-1.4	-1.4	-1.3	-1.3	Leighton and Calo (1981)
c1ccc(Cl)cc1	108-90-7	V	-0.6	-0.3	-0.5	-0.6	Staudinger and Roberts (1996)
c1ccccc1C(Cl)	100-44-7	V	0.4	0.7	0.5	-0.3	Meylan and Howard (2000)
C(Br)	74-83-9	T	-0.8	-0.9	-0.5	-0.9	Meylan and Howard (2000)
CC(Br)	74-96-4	V	-0.9	-1.0	-0.5	-1.0	Hine and Moorkerjee (1975)
CCCC(Br)	109-65-9	T	-1.3	-1.3	-0.8	-1.3	Hoff et al. (1993)
c1ccc(Br)cc1	108-86-1	T	-0.3	-0.2	-0.2	-0.3	Hansen et. al (1995)
CC(C)C(Br)	78-77-3	T	-1.4	-1.3	-0.8	-1.3	Hine and Moorkerjee (1975)
CC(Br)(C)C	507-19-7	T	-1.6	-1.3	-1.2	-1.3	Meylan and Howard (2000)
CC(Br)C	75-26-3	T	-1.0	-1.2	-0.9	-1.2	Meylan and Howard (2000)
CCC(Br)	106-94-5	V	-0.9	-1.2	-0.7	-1.2	Meylan and Howard (2000)
CCCCCCCC(Br)	111-83-1	V	-1.9	-1.8	-1.3	-1.8	Meylan and Howard (2000)
CCCCCCC(Br)	629-04-9	T	-1.7	-1.7	-1.2	-1.7	Meylan and Howard (2000)
CCCCCC(Br)	111-25-1	T	-1.5	-1.5	-1.1	-1.5	Meylan and Howard (2000)
C(I)	74-88-4	V	-0.7	-0.8	-0.9	-0.7	Huntersmith et al. (1983)
C(I)C	75-03-6	T	-0.9	-0.9	-0.9	-0.9	Hine and Moorkerjee (1975)
c1(I)ccccc1	591-50-4	T	-0.1	-0.1	0.3	-0.1	Mackay and Shiu (1981)
C(I)CC	107-08-4	V	-1.0	-1.0	-1.0	-1.0	Meylan and Howard (2000)
C(I)CCC	542-69-8	T	-1.2	-1.2	-1.2	-1.1	Meylan and Howard (2000)
CC(I)C	75-30-9	T	-0.8	-1.0	-1.3	-1.0	Meylan and Howard (2000)
CC(I)CC	513-48-4	T	-1.3	-1.2	-1.3	-1.1	Meylan and Howard (2000)
C(I)CCCC	628-17-1	T	-1.3	-1.3	-1.3	-1.2	Abraham et al. (1994)
C(I)CCCCCC	4282-40-0	T	-1.6	-1.5	-1.5	-1.5	Dunnivant et al. (1988)
O(C=C1)C=C1	110-00-9	T	-0.7	0.5	-0.7	-0.7	Meylan and Howard (2000)
O(CC1)CC1	109-99-9	T	1.1	0.4	1.3	1.1	Sander (1999)
O(CC1)C(C1)C	96-47-9	T	1.0	0.3	1.1	0.9	Sander (1999)
O(C(C1)C)C(C1)C	1003-38-9	V	0.8	0.2	0.9	0.8	Sander (1999)
C1CC-O-CC1	142-68-7	T	0.9	0.3	1.3	0.9	Sander (1999)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
C-O-C=C[b]	107-25-5	T	-0.9	0.0	-1.2	-0.8	Meylan and Howard (2000)
CC(C)C-O-C=C[b]	109-53-5	T	-0.5	-0.4	-1.6	-1.1	Meylan and Howard (2000)
CCCC(=O)-O-CC[b]	105-54-4	V	0.3	0.5	0.3	0.4	Meylan and Howard (2000)
CC(=O)-O-C(C)CC(C)C[b]	108-84-9	T	0.1	0.3	0.1	0.1	Meylan and Howard (2000)
CC(=O)-O-CC=C[b]	591-87-7	T	0.8	1.3	0.9	0.6	Meylan and Howard (2000)
CCCCC(=O)CC[b]	106-35-4	T	0.9	0.9	0.5	0.8	Meylan and Howard (2000)
CCCCCC(=O)CC[b]	106-68-3	V	0.8	0.8	0.4	0.7	Meylan and Howard (2000)
Difunctional							
CC(=O)-O-C(=O)C	108-24-7	T	2.3	1.9	3.5	1.5	Meylan and Howard (2000)
CC(C)-O-CC(O)	109-59-1	V	3.0	3.3	2.9	4.1	Hilal et al. (2008)
CCCC(O)C(C(O))CC	94-96-2	T	4.8	4.9	4.9	3.2	Hilal et al. (2008)
C(O)CCCC(O)	111-29-5	T	6.6	6.3	6.2	3.5	Hilal et al. (2008)
C(O)CCC(O)	110-63-4	T	6.3	6.5	5.7	3.6	Hilal et al. (2008)
C(O)CC(O)	504-63-2	V	6.0	5.5	5.4	3.8	Hilal et al. (2008)
CC(=O)C(N(=O)(=O))	10230-68-9	T	3.0	2.6	4.3	4.6	Hilal et al. (2008)
CC(O)C(N(=O)(=O))	3156-73-8	T	4.0	4.1	4.4	5.6	Hilal et al. (2008)
CCC(N(=O)(=O))C(O)	609-31-4	V	3.8	4.0	4.3	5.4	Hilal et al. (2008)
CC(O)C(N(=O)(=O))C	6270-16-2	T	4.0	4.0	4.3	5.4	Hilal et al. (2008)
CC(N(=O)(=O))C(O)	2902-96-7	T	3.7	4.1	4.4	5.6	Hilal et al. (2008)
C(O)C(N(=O)(=O))	625-48-9	T	4.6	4.3	4.5	5.7	Hilal et al. (2008)
C-O-CC(C)-O-C(=O)C	108-65-6	T	2.4	2.4	2.2	2.4	Hilal et al. (2008)
CCCC-O-CC(O)	111-76-2	V	3.2	3.2	2.9	4.0	Hilal et al. (2008)
CCC-O-CC(O)	2807-30-9	T	3.3	3.3	3.0	4.1	Hilal et al. (2008)
CC(=O)CC(C)-O-C	*n.a.*	T	2.7	2.0	2.6	3.0	Hilal et al. (2008)
C(=O)(O)CCCC(=O)(O)	110-94-1	V	8.3	8.7	9.6	8.1	Hilal et al. (2008)
CC-O-CC(O)	110-80-5	T	3.5	3.4	3.1	4.2	Hilal et al. (2008)
C-O-CC(O)	109-86-4	T	3.6	3.5	3.3	4.4	Hilal et al. (2008)
C(O)(OO)	27828-51-9	T	6.2	6.2	4.2	6.6	O'Sullivan et al. (1996)
c1cc(O)c(O)cc1	120-80-9	T	5.5	5.9	5.2	7.2	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
c1c(O)ccc(O)c1	123-31-9	V	7.3	6.5	7.1	7.2	Meylan and Howard (2000)
C-O-C-O-C	109-87-5	T	0.8	1.1	1.2	1.3	Meylan and Howard (2000)
CC-O-C-O-CC	462-95-3	T	1.2	0.9	1.2	1.0	Meylan and Howard (2000)
CC(=O)C(=O)C	431-03-8	V	1.9	3.3	3.1	3.7	Betterton (1991)
O=CC=O	107-22-2	T	5.6	6.5	5.3	3.4	Zhou and Mopper (1990)
CC(=O)C(=O)	78-98-8	V	4.5	4.8	4.7	3.6	Zhou and Mopper (1990)
C(O)C(=O)	141-46-8	V	4.6	3.5	5.9	2.0	Betterton and Hoffmann (1988)
C(=O)(O)C(=O)(O)	144-62-7	T	6.8	6.7	6.3	7.6	Gaffney et al. (1987)
C(=O)(O)CC(=O)(O)	141-82-2	T	6.6	7.4	8.8	8.4	Meylan and Howard (2000)
C(=O)(O)CCCCC(=O)(O)	124-04-9	T	8.3	8.6	9.7	8.0	Meylan and Howard (2000)
CC(=O)CC(=O)-O-C	105-45-3	T	3.6	3.1	3.4	3.9	Meylan and Howard (2000)
CC(=O)CC(=O)-O-CC	141-97-9	V	2.9	2.9	3.3	3.8	Meylan and Howard (2000)
CC-O-C(=O)-O-CC	105-58-8	T	1.0	1.8	0.6	0.0	Meylan and Howard (2000)
CC-O-C(=O)CC(=O)-O-CC	105-53-3	T	2.7	2.3	2.7	3.1	Meylan and Howard (2000)
CC(=O)-O-CC-O-C(=O)C	111-55-7	T	4.1	3.2	3.2	3.3	Meylan and Howard (2000)
C-O-C(=O)C(=O)-O-C	553-90-2	T	2.5	1.8	3.2	2.6	Meylan and Howard (2000)
C-O-C(=O)C=CC(=O)-O-C	624-48-6	V	3.1	3.1	3.6	3.9	Meylan and Howard (2000)
CC-O-C(=O)CCC(=O)-O-CC	123-25-1	T	3.3	3.6	2.7	3.0	Meylan and Howard (2000)
CCCC-O-C(=O)C=CC(=O)-O-CCCC	105-76-0	V	3.4	2.4	2.7	3.1	Meylan and Howard (2000)
C-O-C(=O)c1ccccc1C(=O)-O-C	131-11-3	T	4.0	3.7	4.6	3.7	Meylan and Howard (2000)
c1cc(N(=O)(=O))cc(N(=O)(=O))c1C	121-14-2	T	4.3	4.0	3.2	4.0	Meylan and Howard (2000)
c1cc(N(=O)(=O))cc(N(=O)(=O))c1	99-65-0	T	4.3	4.1	3.2	4.1	Meylan and Howard (2000)
C(ON(=O)(=O))C(ON(=O)(=O))	628-96-6	V	1.9	2.0	3.0	3.2	Fischer and Ballschmiter (1998)
CC(ON(=O)(=O))C(ON(=O)(=O))	6423-43-4	V	1.5	1.9	2.5	3.0	Fischer and Ballschmiter (1998)
C(ON(=O)(=O))CC(ON(=O)(=O))	3457-90-7	T	2.1	2.1	2.6	3.0	Fischer and Ballschmiter (1998)
CCC(ON(=O)(=O))C(ON(=O)(=O))	20820411	V	1.3	1.7	2.2	2.9	Fischer and Ballschmiter (1998)
CC(ON(=O)(=O))CC(ON(=O)(=O))	6423-44-5	T	1.8	2.0	2.2	2.9	Fischer and Ballschmiter (1998)
C(ON(=O)(=O))CCC(ON(=O)(=O))	3457-91-8	T	2.2	2.0	2.5	2.9	Fischer and Ballschmiter (1998)
CC(ON(=O)(=O))C(ON(=O)(=O))C	6423-45-6	T	1.1	1.7	2.2	2.9	Fischer and Ballschmiter (1998)
CCCC(ON(=O)(=O))C(ON(=O)(=O))	*n.a.*	T	1.1	1.6	2.1	2.8	Fischer and Ballschmiter (1998)
CC(ON(=O)(=O))CCC(ON(=O)(=O))	*n.a.*	T	1.6	1.9	2.1	2.8	Fischer and Ballschmiter (1998)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
C(ON(=O)(=O))CCCC(ON(=O)(=O))	3457-92-9	T	2.1	2.0	2.3	2.8	Fischer and Ballschmiter (1998)
CC(ON(=O)(=O))CC(ON(=O)(=O))C	101421-04-9	V	1.3	1.8	1.9	2.8	Fischer and Ballschmiter (1998)
CCCCC(ON(=O)(=O))C(ON(=O)(=O))	*n.a.*	T	1.0	1.5	1.9	2.7	Fischer and Ballschmiter (1998)
C(ON(=O)(=O))CCCCC(ON(=O)(=O))	*n.a.*	T	2.2	1.8	2.1	2.7	Fischer and Ballschmiter (1998)
CC(ON(=O)(=O))CCC(ON(=O)(=O))C	*n.a.*	V	1.5	1.8	1.8	2.7	Fischer and Ballschmiter (1998)
C1CC(ON(=O)(=O))C(ON(=O)(=O))CC1	*n.a.*	T	2.1	2.1	2.6	3.0	Fischer and Ballschmiter (1998)
C1CC(ON(=O)(=O))CC(ON(=O)(=O))C1	*n.a.*	T	2.5	2.3	2.5	3.0	Fischer and Ballschmiter (1998)
C(ON(=O)(=O))CCCCCC(ON(=O)(=O))	*n.a.*	T	2.1	1.7	2.0	2.5	Fischer and Ballschmiter (1998)
C1CCC(ON(=O)(=O))C(ON(=O)(=O))CCC1	*n.a.*	T	1.9	1.8	2.6	2.8	Fischer and Ballschmiter (1998)
CCCCCCC(ON(=O)(=O))C(ON(=O)(=O))	*n.a.*	T	0.7	1.2	1.7	2.4	Fischer and Ballschmiter (1998)
C(ON(=O)(=O))CCCCCCC(ON(=O)(=O))	*n.a.*	T	1.9	1.6	1.9	2.4	Fischer and Ballschmiter (1998)
CCCCCCCCC(ON(=O)(=O))C(ON(=O)(=O))	*n.a.*	T	0.3	1.0	1.4	2.2	Fischer and Ballschmiter (1998)
C(ON(=O)(=O))CCCCCCCCC(ON(=O)(=O))	*n.a.*	T	1.6	1.4	1.7	2.2	Fischer and Ballschmiter (1998)
CC(O)C-O-C	107-98-2	T	3.0	3.4	3.3	4.2	Johanson and Dynesius (1988)
CC(=O)C(=O)(O)	127-17-3	T	5.5	5.2	8.3	5.7	Khan et al. (1995)
CC-O-CC-O-C(=O)C	111-15-9	T	2.5	2.4	2.4	2.4	Johanson and Dynesius (1988)
CC(=O)CC(C)(C)-O-C	107-70-0	V	2.7	1.9	2.3	2.9	Meylan and Howard (2000)
C(O)C(ON(=O)(=O))	16051-48-2	T	4.6	3.6	4.3	5.0	Shepson et al. (1996)
C(O)CC(ON(=O)(=O))	*n.a.*	V	3.9	3.3	4.6	4.9	Kames and Schurath (1995)
CC(O)C(ON(=O)(=O))	20266-65-3	T	4.0	3.5	4.1	4.9	Shepson et al. (1996)
CC(ON(=O)(=O))C(O)	20266-74-4	T	3.7	3.5	4.0	4.9	Shepson et al. (1996)
CC(O)C(ON(=O)(=O))C	147794-10-3	V	4.0	3.4	3.9	4.8	Shepson et al. (1996)
CCC(O)C(ON(=O)(=O))	147794-11-4	T	3.8	3.4	3.9	4.8	Shepson et al. (1996)
CCC(ON(=O)(=O))C(O)	147794-12-5	T	3.8	3.4	3.8	4.8	Shepson et al. (1996)
CC(=O)C(ON(=O)(=O))	6745-71-7	T	3.0	3.4	3.6	3.9	Kames and Schurath (1995)
c1c(C)ccc(O)c1-O-C	93-51-6	V	2.9	3.5	2.5	4.4	Sagebiel et al. (1992)
c1ccccc1C-O-CC(O)	622-08-2	T	3.9	5.2	4.2	5.5	Meylan and Howard (2000)
CC(=O)-O-c1ccccc1C(=O)(O)	50-78-2	V	5.9	4.8	6.7	5.9	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
c1cccc(O)c1C(=O)(O)	69-72-7	T	5.1	5.2	4.7	4.8	Meylan and Howard (2000)
c1ccc(O)cc1-O-C	150-19-6	T	4.2	4.3	4.4	4.5	Meylan and Howard (2000)
c1cc(O)c(N(=O)(=O))cc1	88-75-5	T	2.2	1.6	1.9	2.2	Guo and Brimblecombe (2007)
c1c(O)cc(N(=O)(=O))cc1	554-84-7	T	4.1	5.3	6.1	5.7	Guo and Brimblecombe (2007)
c1c(O)ccc(N(=O)(=O))c1	100-02-7	T	3.9	5.3	5.6	5.7	Guo and Brimblecombe (2007)
c1cccc(N(=O)(=O))c1-O-C	91-23-6	T	3.4	3.1	1.6	2.9	Meylan and Howard (2000)
C1CCC-O-C1C(O)	100-72-1	V	4.8	3.8	4.5	5.3	Meylan and Howard (2000)
c1ccc(O)cc1C(=O)	100-83-4	T	5.6	5.1	6.2	5.8	Meylan and Howard (2000)
c1cc(O)ccc1C(=O)	123-08-0	T	6.3	5.1	5.4	5.8	Meylan and Howard (2000)
c1cccc(O)c1C(=O)	90-02-8	V	2.3	2.8	3.0	2.8	Meylan and Howard (2000)
O(C=C1)C(=C1)C(=O)	98-01-1	V	2.5	1.3	2.8	1.9	Meylan and Howard (2000)
CCC-O-C(=O)c1ccccc1C(=O)-O-CCC	131-16-8	V	3.4	3.2	3.9	3.2	Meylan and Howard (2000)
CC(F)(F)	75-37-6	V	-1.3	-1.3	-1.8	-2.6	Zheng et al. (1997)
C(F)C(=O)(O)	144-49-0	V	4.9	4.8	5.0	3.0	Bowden et al. (1998)
C(Cl)(Cl)	75-09-2	T	-0.4	-0.5	0.1	-1.0	Staudinger and Roberts (1996)
CC(Cl)(Cl)	75-34-3	T	-0.8	-0.7	-0.5	-1.1	Staudinger and Roberts (1996)
C(Cl)C(Cl)	107-06-2	V	-0.1	-0.3	0.0	-1.1	Staudinger and Roberts (1996)
CC(Cl)C(Cl)	78-87-5	T	-0.5	-0.4	-0.3	-1.2	Staudinger and Roberts (1996)
C(Cl)(Cl)=C	75-35-4	T	-1.5	-1.2	-1.8	-1.5	Staudinger and Roberts (1996)
C(Cl)=C(Cl)	156-59-2	T	-0.6	-1.2	-1.3	-1.5	Staudinger and Roberts (1996)
C(Cl)=C(Cl)	156-59-2	T	-1.0	-1.2	-1.3	-1.5	Staudinger and Roberts (1996)
C(Cl)C=C(Cl)	542-75-6	T	-0.2	-0.4	-0.2	-1.4	Wright et al. (1992)
C(Cl)C(Cl)=C	78-88-6	T	-0.6	-0.4	-0.2	-1.4	Pearson and McConnell (1975)
CC(=O)C(Cl)	78-95-5	V	1.8	2.2	2.1	1.8	Betterton (1991)
C(Cl)C(=O)(O)	79-11-8	V	5.0	5.1	5.2	3.7	Bowden et al. (1998)
c1cc(Cl)c(Cl)cc1	95-50-1	T	-0.3	-0.2	-0.2	-0.5	Staudinger and Roberts (1996)
c1cc(Cl)cc(Cl)c1	541-73-1	V	-0.4	-0.2	-0.3	-0.5	Meylan and Howard (2000)
c1c(Cl)ccc(Cl)c1	106-46-7	V	-0.4	-0.2	-0.2	-0.5	Meylan and Howard (2000)
C(Cl)(F)	593-70-4	T	-0.8	-0.9	-0.4	-1.7	Wilhelm et al. (1977)
C(Br)(Br)	74-95-3	T	0.0	-0.2	0.7	0.0	Moore et al. (1995)
C(Br)C(=O)(O)	79-08-3	T	5.2	5.3	5.4	4.2	Bowden et al. (1998)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
c1cc(Br)cc(Br)c1	108-36-1	T	-0.3	0.1	0.3	0.1	Mackay and Shiu (1981)
c1c(Br)ccc(Br)c1	106-37-6	T	-0.3	0.1	0.4	0.1	Mackay and Shiu (1981)
c1c(O)ccc(Br)c1	106-41-2	T	3.8	3.3	3.4	3.7	Parsons et al. (1971)
c1c(Cl)ccc(Br)c1	106-39-8	V	-0.2	-0.1	0.1	-0.2	Mackay and Shiu (1981)
C(I)(I)	75-11-6	V	0.4	0.0	0.8	0.4	Moore et al. (1995)
C(Cl)(I)	593-71-5	V	-0.1	-0.3	0.4	-0.3	Moore et al. (1995)
C(O)C(=O)(O)	79-14-1	T	4.4	5.1	6.5	4.1	Ip et al. (2009)
C(=O)C(=O)(O)	298-12-4	T	4.0	6.9	10.4	5.5	Ip et al. (2009)
CC(O)C(=O)(O)	50-21-5	T	4.1	5.0	6.0	4.0	Meylan and Howard (2000)
C(=O)(O)CCC(=O)(O)	110-15-6	T	9.4	8.7	8.4	8.3	Meylan and Howard (2000)
O(C=C1)C(=C1)CO	98-00-0	V	4.1	3.8	3.6	3.7	Hilal et al. (2008)
C1-O-CC-O-C1	123-91-1	T	2.3	1.9	3.1	2.2	Cabani et al. (1971)
C(O)C(O)[b]	107-21-1	T	6.5	5.9	4.7	3.9	Bone et al.(1983)
c1cc(O)c(N(=O)(=O))cc1C[b]	119-33-5	T	1.7	1.5	1.8	2.1	Tremp et al. (1993)
c1cc(N(=O)(=O))c(O)cc1C[b]	700-38-9	V	1.8	1.5	1.9	2.1	Tremp et al. (1993)
c1c(O)ccc(N(=O)(=O))c1C[b]	2581-34-2	V	4.7	5.2	5.6	5.6	Tremp et al. (1993)
c1ccc(N(=O)(=O))c(O)c1C[b]	13073-29-5	T	1.4	1.5	2.6	2.1	Tremp et al. (1993)
CCCC-O-CC-O-C(=O)C[b]	112-07-2	T	2.2	2.1	2.2	2.2	Meylan and Howard (2000)
CCCC-O-C(=O)C(O)C[b]	138-22-7	V	2.6	2.2	3.1	1.1	Meylan and Howard (2000)
CC(=O)CC(=O)C[b]	123-54-6	T	2.5	3.6	3.4	4.3	Meylan and Howard (2000)
c1cc(O)c(N(=O)(=O))cc1C(C)CC[b]	3555-18-8	T	1.3	1.1	1.6	1.7	Schwarzenbach et al (1988)
Multifunctional							
C(Cl)C(O)C(Cl)	96-23-1	V	2.8	3.3	3.7	3.2	Hilal et al. (2008)
C(O)CC-O-CC(O)	*n.a.*	V	6.5	6.7	6.7	5.6	Hilal et al. (2008)
CC(=O)-O-CC(-O-C(=O)C)C-O-C(=O)C	102-76-1	T	4.9	5.3	4.4	5.8	Meylan and Howard (2000)
C(ON(=O)(=O))C(ON(=O)(=O))C(ON(=O)(=O))	55-63-0	T	4.0	3.7	4.6	5.6	Meylan and Howard (2000)
CCCC-O-CC-O-CC-O-C(=O)C	124-17-4	T	3.8	3.8	3.9	4.0	Meylan and Howard (2000)
C(ON(=O)(=O))C-O-CC(ON(=O)(=O))	693-21-0	T	3.4	3.7	4.1	5.0	Meylan and Howard (2000)
c1ccc(-O-C)c(O)c1-O-C	91-10-1	V	3.6	4.9	4.7	5.7	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
C-O-c1c(O)ccc(c1)C(=O)	121-33-5	T	5.7	5.7	4.5	7.1	Meylan and Howard (2000)
c1c(N(=O)(=O))cc(N(=O)(=O))c(O)c1C(C)C	*n.a.*	V	3.3	3.4	4.8	4.2	Meylan and Howard (2000)
C(F)(F)(F)	75-46-7	T	-1.8	-1.8	-1.7	-2.8	Wilhelm et al. (1977)
C(F)(F)(F)C(F)	811-97-2	V	-1.7	-1.6	-1.9	-3.2	Wilhelm et al. (1977)
C(O)C(F)(F)(F)	75-89-8	T	1.8	1.6	1.4	1.5	Rochester and Symonds(1973)
CC(O)C(F)(F)(F)	374-01-6	T	1.7	1.5	1.2	1.4	Rochester and Symonds (1973)
C(O)C(F)(F)C(F)(F)	76-37-9	T	2.2	2.1	1.6	1.1	Rochester and Symonds (1973)
C(O)C(F)(F)C(F)(F)(F)	422-05-9	T	1.7	1.3	1.4	0.8	Rochester and Symonds (1973)
C(F)(F)(F)C(O)C(F)(F)(F)	920-66-1	T	1.4	1.2	0.3	0.5	Rochester and Symonds (1973)
CC(=O)C(F)(F)(F)	421-50-1	T	2.1	2.7	1.0	0.4	Betterton (1991)
C(F)(F)C(=O)(O)	381-73-7	T	4.5	4.7	4.0	2.7	Bowden et al. (1998)
C(F)(F)(F)C(=O)(O)	76-05-1	T	3.9	3.8	1.2	2.4	Bowden et al. (1998)
c1ccccc1C(F)(F)(F)	98-08-8	T	-1.2	-0.1	-0.9	-1.7	Mackay and Shiu (1981)
C(Cl)(Cl)(Cl)	67-66-3	T	-0.6	-0.6	-0.5	-0.5	Staudinger and Roberts (1996)
CC(Cl)(Cl)(Cl)	71-55-6	T	-1.2	-0.8	-1.1	-0.6	Staudinger and Roberts (1996)
C(Cl)(Cl)C(Cl)	79-00-5	V	0.0	0.1	0.2	-0.6	Staudinger and Roberts (1996)
C(Cl)(Cl)(Cl)C(Cl)	630-20-6	V	-0.4	-0.1	-0.4	-0.2	Wright et al. (1992)
C(Cl)(Cl)C(Cl)(Cl)	79-34-5	V	0.4	0.6	0.3	-0.2	Staudinger and Roberts (1996)
C(Cl)(Cl)(Cl)C(Cl)(Cl)	76-01-7	T	-0.3	0.3	-0.3	0.3	Staudinger and Roberts (1996)
C(Cl)C(Cl)C(Cl)	96-18-4	T	0.5	0.4	0.6	-0.7	Staudinger and Roberts (1996)
C(Cl)C(Cl)CCCCCCC(Cl)C(Cl)	*n.a.*	T	0.8	0.8	0.6	-1.2	Drouillard et al. (1998)
C(Cl)C(Cl)CCCCCCCC(Cl)C(Cl)	*n.a.*	T	1.2	0.7	0.5	-1.3	Drouillard et al. (1998)
C(Cl)(Cl)=C(Cl)	79-01-6	V	-1.0	-1.6	-1.7	-1.4	Staudinger and Roberts (1996)
C(Cl)(Cl)(Cl)C(=O)	75-87-6	T	5.5	5.1	4.5	2.5	Betterton and Hoffmann (1988)
C(Cl)(Cl)C(=O)(O)	79-43-6	V	5.1	5.4	4.8	4.2	Bowden et al. (1998)
C(Cl)(Cl)(Cl)C(=O)(O)	76-03-9	V	4.9	5.0	2.6	4.6	Sander (1999)
c1cc(Cl)c(Cl)c(Cl)c1	87-61-6	V	-0.1	-0.1	-0.2	-0.3	Meylan and Howard (2000)
c1c(Cl)cc(Cl)cc1(Cl)	108-70-3	T	-0.3	-0.1	-0.3	-0.3	Meylan and Howard (2000)
c1c(Cl)c(Cl)c(Cl)c(Cl)c1	634-66-2	T	0.1	-0.1	-0.1	-0.2	Meylan and Howard (2000)
c1c(Cl)c(Cl)c(Cl)cc1(Cl)	634-90-2	T	-0.2	-0.1	-0.2	-0.2	Meylan and Howard (2000)
c1c(Cl)c(Cl)cc(Cl)c1(Cl)	95-94-3	T	0.0	-0.1	-0.1	-0.2	Meylan and Howard (2000)

SMILES	CAS Number	Subset[a]	log H^*_{exp}	log H^*_{est}			Reference
				GROMHE	*SPARC*	$HWIN_b$	
c1c(Cl)c(Cl)c(Cl)c(Cl)c1(Cl)	608-93-5	V	0.2	0.0	-0.2	-0.1	Meylan and Howard (2000)
C(Cl)(F)(F)	75-45-6	T	-1.4	-1.4	-1.2	-2.0	Wilhelm et al. (1977)
C(Cl)(F)(F)C(=O)(O)	76-04-0	T	4.4	4.0	1.7	3.1	Sander (1999)
C(Br)(Br)(Br)	75-25-2	T	0.2	-0.3	-0.2	0.9	Staudinger and Roberts (1996)
C(Br)(Br)C(=O)(O)	631-64-1	T	5.4	5.6	4.8	5.1	Bowden et al. (1998)
C(Br)(Br)(Br)C(=O)(O)	75-96-7	V	5.5	5.3	3.0	6.1	Bowden et al. (1998)
C(Cl)(Cl)(Br)	75-27-4	V	-0.4	-0.5	-0.4	0.0	Staudinger and Roberts (1996)
c1cc(O)c(N(=O)(=O))cc1-O-C[b]	1568-70-3	T	2.6	2.8	4.1	3.4	Tremp et al. (1993)
c1c(O)c(N(=O)(=O))cc(N(=O)(=O))c1[b]	51-28-5	T	4.0	3.9	4.8	4.6	Tremp et al. (1993)
O-c(ccc1C=O)c(c1)N(=O)(=O)[b]	3011-34-5	T	2.9	3.6	4.3	4.8	Schwarzenbach et al (1988)
c1c(N(=O)(=O))cc(O)c(N(=O)(=O))c1[b]	329-71-5	V	3.1	3.9	4.7	4.6	Schwarzenbach et al (1988)

n.a.: not available.

a : T stands for Training dataset and V for Validation dataset.

b : Original value at 293K, calculated at 298K using ΔH_{solv}= 50 kJ mol^{-1}.

Table S2 : Hydration constants from literature and estimated using our SAR for aldehydes and ketones in log unit.

SMILES	CAS Number	$K_{hyd,exp}$	$K_{hyd,est}$	Reference
CC(=O)	75-07-0	0,08	0,08	Buschmann (1980)
CCC(=O)	123-38-6	0,09	0,08	Buschmann (1980)
CCCC(=O)	123-72-8	-0,24	0,08	Buschmann (1980)
CCCCC(=O)	110-62-3	-0,26	0,08	Sham and Joens (1995)
CCCCCC(=O)	66-25-1	-0,31	0,08	Sham and Joens (1995)
CC(C)C(=O)	78-84-2	-0,29	0,08	Sham and Joens (1995)
CC(C)(C)C(=O)	630-19-3	-0,64	0,08	Le Henaff (1968)
C(Cl)C(=O)	107-20-0	1,46	1,27	Le Henaff (1968)
CC(Cl)(C)C(=O)	917-93-1	1,19	1,27	Le Henaff (1968)
CCC(Cl)C(=O)	2883-255-5	1,61	1,27	Le Henaff (1968)
CCCCCC(Cl)C(=O)	6393-808-9	1,28	1,27	Le Henaff (1968)
C(Cl)(Cl)(Cl)C(=O)	75-87-6	4,45	3,65	Le Henaff (1968)
CCCCCC(Br)(Br)C(=O)	n.a.	1,44	2,61	Le Henaff (1968)
CCC(Br)C(=O)	2476-497-4	1,12	1,35	Le Henaff (1968)
C(O)C(=O)	141-46-8	0,95	0,87	Buschmann (1980)
CC(O)C(=O)	3913-65-3	1,36	0,87	Buschmann (1980)
C(=O)(O)C(=O)	298-12-4	3,04	2,72	Tury'an (1998)
C(=O)C(=O)	107-22-2	2,24	2,8	Montoya and Mellado (1994)
C(O)(O)C(=O)	631-59-4	2,31	1,65	Montoya and Mellado (1994)
C(=O)CCCC(=O)	111-30-8	0,57	0,26	Malik (2000)
CC(=O)C(=O)	78-98-8	3,14	2,37	Montoya and Mellado (1994)
c1ccccc1C(=O)C(=O)	1074-12-0	2,6	2,37	Montoya and Mellado (1994)
CC(=O)C	67-64-1	-2,85	-2,42	Guthrie (1978)
CC(=O)C(F)	430-51-3	-0,78	-1,03	Guthrie (1978)
CC(=O)C(Cl)	78-95-5	-1,04	-1,23	Le Henaff (1968)
CC(=O)C(Br)	598-31-2	-1,15	-1,16	Le Henaff (1968)
CC(=O)C(Cl)(Cl)	513-88-2	0,45	-0,04	Guthrie (1975)
C(Cl)C(=O)C(Cl)	534-07-6	0,62	-0,04	Guthrie (1975)
C(Br)C(=O)C(Br)	816-39-7	0,27	0,11	Buschmann (1980)
CC(=O)C(F)(F)(F)	421-50-1	1,54	1,76	Buschmann (1980)
C(F)(F)(F)C(=O)C(F)(F)(F)	684-16-2	6,08	5,94	Guthrie (1975)
CC(=O)CC(=O)C(F)(F)(F)	367-57-7	1,89	2,67	Guthrie (1975)
CC(=O)C(=O)(O)	127-17-3	0,47	0,21	Kozlowski and Zuman (1987)
CCC(=O)C(=O)(O)	600-18-0	0,23	0,21	Buschmann (1980)
CC(C)C(=O)C(=O)(O)	759-05-7	0,05	0,21	Cooper et al. (1975)
CCC(C)C(=O)C(=O)(O)	1460-34-0	0,18	0,21	Cooper et al. (1975)
CC(C)CCC(=O)C(=O)(O)	n.a.	-0,95	0,21	Cooper et al. (1975)
C(=O)(O)CC(=O)C(=O)(O)	328-42-7	0,85	1,27	Kozlowski and Zuman (1987)
C(=O)(O)CCC(=O)C(=O)(O)	328-50-7	0,34	0,63	Kozlowski (1987)
C(=O)(O)CCCC(=O)C(=O)(O)	689-31-6	0,23	0,38	Cooper et al. (1975)

SMILES	CAS Number	$K_{hyd,exp}$	$K_{hyd,est}$	Reference
c1ccccc1CC(=O)C(=O)(O)	156-06-9	0,6	0,21	Cooper et al. (1975)
CCOC(=O)C(=O)CC(=O)(O)	n.a.	0,89	1,16	Kozlowski and Zuman (1987)
CCOC(=O)CCC(=O)C(=O)OCC	5965-53-7	0,39	0,52	Kozlowski (1987)
CCOC(=O)CC(=O)C(=O)OCC	108-56-5	1,15	1,12	Kozlowski and Zuman (1987)
C(=O)(O)C(=O)C(=O)(O)	473-90-5	2,00	2,85	Le Henaff (1968)
CC(=O)C(=O)C	431-03-8	0,22	-0,13	Zuman (2002)
CCC(=O)C(=O)CC	4437-51-8	0,01	-0,13	Montoya and Mellado (1994)
CCC(=O)C(=O)C	600-14-6	0,10	-0,13	Buschmann (1982)
CC(=O)C(=O)OC	600-22-6	0,41	0,11	Buschmann (1982)
CC(=O)C(=O)OCC	617-35-6	0,41	0,11	Buschmann (1982)
C(F)C(=O)C(=O)(O)	n.a.	2,58	1,6	Hurley (1979)
c1ccccc1C(=O)	100-52-7	-2,10	-1,5	McClelland (1983)
c1cc(Cl)ccc1C(=O)	104-88-1	-1,80	-1,38	McClelland (1983)
c1ccc(Cl)cc1C(=O)	587-04-2	-1,66	-1,32	McClelland (1983)
c1cc(Cl)c(Cl)cc1C(=O)	6287-38-3	-1,35	-1,2	McClelland (1983)
C(F)(F)(F)c1ccc(C(=O))cc1	455-19-6	-1,26	-1,5	McClelland (1983)
c1ccc(N(=O)(=O))cc1C(=O)	99-61-6	-0,96	-1,13	McClelland (1983)
c1cc(N(=O)(=O))ccc1C(=O)	555-16-8	-0,77	-1,11	McClelland (1983)
c1cc(Cl)c(N(=O)(=O))cc1C(=O)	1658-834-4	-0,74	-1,01	McClelland (1983)
c1c(N(=O)(=O))cc(N(=O)(=O))cc1C(=O)	1419-318-1	0,32	-0,76	McClelland (1983)
c1cc(Cl)c(C(=O))c(N(=O)(=O))c1	6361-22-4	-0,47	0,12	Guthrie (2000)

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