Supplementary material

August 18, 2011

1 Data collection for the development of EVAPORATION

Table 1. SMILES formula, names, and references of the molecules on which EVAPORATION is based. The data type numbers are explained in Table 2.

SMILES	name	data type	reference
hydrocarbons			
CC	ethane	1	[1]
CCC	propane	1	[1]
CCCC	butane	1	[1]
CCCCC	pentane	1	[1]
CCCCCC	hexane	1	[1]
CCCCCCC	heptane	1	[1]
CCCCCCCC	octane	1	[1]
CCCCCCCCC	nonane	1	[1]
CCCCCCCCCC	decane	1	[1]
CCCCCCCCCCC	undecane	1	[1]
CCCCCCCCCCCC	dodecane	1	[1]
CCCCCCCCCCCCC	tridecane	1	[1]
CCCCCCCCCCCCCC	tetradecane	1	[1]
CC(C)C	2-methylpropane	1	[1]
CC(C)CC	2-methylbutane	1	[2]
CC(C)(C)C	2,2-dimethylpropane	1	[2]
CC(C)CCC	2-methylpentane	1	[2]
CCC(C)CC	3-methylpentane	1	[2]
CC(C)(C)CC	2,2-dimethylbutane	1	[2]
CC(C)C(C)C	2,3-dimethylbutane	1	[2]
CC(C)CCCC	2-methylhexane	1	[2]
CCC(C)CCC	3-methylhexane	1	[2]
CCC(CC)CC	3-ethylpentane	1	[2]
CC(C)(C)CCC	2,2-dimethylpentane	1	[2]

SMILES	name	data type	reference
CCC(C)(C)CC	3,3-dimethylpentane	1	[2]
CC(C)C(C)CC	2,3-dimethylpentane	1	[2]
CC(C)CC(C)C	2,4-dimethylpentane	1	[2]
CC(C)(C)C(C)C	2,2,3-trimethylbutane	1	[2]
CC(C)CCCCC	2-methylheptane	1	[2]
CCC(C)CCCC	3-methylheptane	1	[2]
CCCC(C)CCC	4-methylheptane	1	[3]
CCC(CC)CCC	3-ethylhexane	1	[2]
CC(C)(C)CCCC	2,2-dimethylhexane	1	[2]
CC(C)CC(C)CC	2,4-dimethylhexane	1	[2]
CC(C)CCC(C)C	2,5-dimethylhexane	1	[2]
CCC(C)(C)CCC	3,3-dimethylhexane	1	[2]
CCC(C)C(C)CC	3,4-dimethylhexane	1	[2]
CC(C)(C)CC(C)C	2,2,4-trimethylpentane	1	[2]
CC(C)C(C)C(C)C	2,3,4-trimethylpentane	1	[2]
CC(C)(C)C(C)(C)C	2,2,3,3-tetramethylbutane	1	NIST (Scott)
CC(C)CCCCCC	2-methyloctane	1	[2]
CCC(C)CCCCC	3-methyloctane	1	[2]
CCCC(C)CCCC	4-methyloctane	1	[2]
CC(C)CCCC(C)C	2,6-dimethylheptane	1	[2]
CCC(C)(C)CCCC	3,3-dimethylheptane	1	[3]
CCC(C)CC(C)CC	3,5-dimethylheptane	1	[3]
CC(C)CC(CC)CC	4-ethyl-2-methylhexane	1	[3]
CC(C)(C)CC(C)(C)C	2,2,4,4-tetramethylpentane	1	[2]
CC(C)CCCCCCC	2-methylnonane	1	[2]
CCC(C)CCCCCC	3-methylnonane	1	[2]
CCCC(C)CCCCC	4-methylnonane	1	[2]

SMILES	name	data type	reference
CCCCC(C)CCCC	5-methylnonane	1	[2]
CC(C)CCCCC(C)C	2,7-dimethyloctane	1	[3]
CC(C)CC(C)CC(C)C	2,4,6-trimethylheptane	1	[4]
CC(C)(C)CC(C)(C)CC	2,2,4,4-tetramethylhexane	1	[3]
CC(C)(C)CCC(C)(C)C	2,2,5,5-tetramethylhexane	1	[3]
C1CCC1	cyclobutane	1	[1]
C1CCCC1	cyclopentane	1	[2]
C1CCCCC1	cyclohexane	1	[2]
CC1CCCC1	methylcyclopentane	1	[3]
C1CCCCCC1	cycloheptane	1	[2]
CC1CCCCC1	methylcyclohexane	1	[2]
CCC1CCCC1	ethylcyclopentane	1	[2]
CC1CC(C)CC1	cis-1,3-dimethylcyclopentane	1	[2]
CC1CC(C)CC1	trans-1,3-dimethylcyclopentane	1	[2]
C1CCCCCCC1	cyclooctane	1	[2]
CCC1CCCCC1	ethylcyclohexane	1	[3]
CC1(C)CCCCC1	1,1-dimethylcyclohexane	1	[3]
CC1C(C)CCCC1	cis-1,2-dimethylcyclohexane	1	[2]
CC1C(C)CCCC1	trans-1,2-dimethylcyclohexane	1	[2]
CC1CC(C)CCC1	cis-1,3-dimethylcyclohexane	1	[2]
CC1CC(C)CCC1	trans-1,3-dimethylcyclohexane	1	[2]
CC1CCC(C)CC1	cis-1,4-dimethylcyclohexane	1	[2]
CC1CCC(C)CC1	trans-1,4-dimethylcyclohexane	1	[3]
C1CCCC(C1)C2CCCCC2	bicyclohexyl	1	[3]
C=C	ethene	1	[1]
C=CC	propene	1	[1]
C=CCC	1-butene	1	[1]

SMILES	name	data type	reference
CC=CC	cis-2-butene	1	[1]
CC=CC	trans-2-butene	1	[1]
C=CCCC	1-pentene	1	[2]
CC=CCC	cis-2-pentene	1	[2]
CC=CCC	trans-2-pentene	1	[2]
C=CCCCC	1-hexene	1	[2]
CC=CCCC	cis-2-hexene	1	[2]
CC=CCCC	trans-2-hexene	1	[2]
CCC=CCC	cis-3-hexene	1	[2]
CCC=CCC	trans-3-hexene	1	[2]
CC=CC=CC	cis,trans-2,4-hexadiene	1	[2]
CC=CC=CC	trans,trans-2,4-hexadiene	1	[2]
C=CCCCCC	1-heptene	1	[2]
CC=CCCCC	trans-2-heptene	1	[2]
C=CCCCCCC	1-octene	1	[2]
CC=CCCCCC	2-octene	1	[2]
CCCC=CCCC	4-octene	1	[2]
C=CCCCCCCC	1-nonene	1	[2]
C=CCCCCCCCC	1-decene	1	[2]
C=CCCCCCCCCC	1-undecene	1	[2]
C=C(C)C	2-methylpropene	1	[1]
CC(C)=CC	2-methyl-2-butene	1	[2]
C=C(C)CC	2-methyl-1-butene	1	[2]
C=CC(C)C	3-methyl-1-butene	1	[2]
CC(C)=CCC	2-methyl-2-pentene	1	[2]
C=CC(C)(C)C	3,3-dimethyl-1-butene	1	[2]
CC(C)=C(C)C	2,3-dimethyl-2-butene	1	[2]

SMILES	name	data type	reference
C=C(C)CCC	2-methyl-1-pentene	1	[2]
C=CCC(C)C	4-methyl-1-pentene	1	[2]
CC=C(C)CC	3-methyl-cis-2-pentene	1	[2]
CC=CC(C)C	4-methyl-cis-2-pentene	1	[2]
CC=CC(C)C	4-methyl-trans-2-pentene	1	[2]
C=C(C)CCCC	2-methyl-1-hexene	1	[2]
C=CC(C)CCC	3-methyl-1-hexene	1	[2]
C=CCC(C)CC	4-methyl-1-hexene	1	[2]
CC(C)=CCCC	2-methyl-2-hexene	1	[3]
C=C(C)CCCCC	2-methyl-1-heptene	1	[4]
CC(C)=CCCCC	2-methyl-2-heptene	1	[3]
C=C(C)CCCCCC	2-methyl-1-octene	1	[4]
C1=CCCC1	cyclopentene	1	[2]
C1=CC=CC1	cyclopentadiene	1	[3]
CC1=CC=CC1	methylcyclopentadiene	1	[3]
C1=CCCCC1	cyclohexene	1	[2]
CC1=CCCC1	1-methylcyclopentene	1	[3]
C1=CC(C)CC1	3-methylcyclopentene	1	[3]
CC1=CCCCC1	1-methylcyclohexene	1	[3]
C1=CCC(C)CC1	4-methylcyclohexene	1	[3]
C1=CCCCCC1	cycloheptene	1	[3]
CC1(C)C(=C)C2CC1CC2	camphene	1	[2]
C=C(C)C1CC=C(C)CC1	d-limonene	1	[2]
CC1(C)C2C(C)=CCC1C2	a-pinene	1	[2]
CC1(C)C2C(=C)CCC1C2	b-pinene	1	[2]
monofunctional			
mononitrates			

SMILES	name	data type	reference
O=N(=O)OC	methylnitrate	1	[5]
O=N(=O)OCC	ethylnitrate	1	[5]
O=N(=O)OCCC	1-propylnitrate	1	[5]
O=N(=O)OC(C)C	2-propylnitrate	1	[5]
O=N(=O)OC(C)=C	2-propenylnitrate	3	[6]
O=N(=O)OC(C)CC	2-butylnitrate	3	[7]
O=N(=O)OC(C)CC	2-butylnitrate	4	[7]
O=N(=O)OCC(C)C	2-methylpropylnitrate	1	[5]
O=N(=O)OC(C)(C)C	t-butylnitrate	4	[8]
O=N(=O)OCC(C)=C	2-methyl-2-propenylnitrate	4	[7]
O=N(=O)OCCCCC	1-pentylnitrate	4	[9]
O=N(=O)OCCCCC	1-pentylnitrate	3	[7]
O=N(=O)OC(C)CCC	2-pentylnitrate	3	[7]
O=N(=O)OCCC(C)C	3-methylbutylnitrate	1	[10]
O=N(=O)OC(C)(C)CC	2-methyl-2-butylnitrate	4	[7]
O=N(=O)OCCCCCC	1-hexylnitrate	4	[6]
O=N(=O)OCCCCCC	1-hexylnitrate	4	[11]
O=N(=O)OCCCCCC	1-hexylnitrate	3	[7]
O=N(=O)OC(C)CCCCC	2-heptylnitrate	4	[7]
O=N(=O)OC(CCC)CCC	4-heptylnitrate	4	[7]
O=N(=O)OCCCCCCCCC	1-octylnitrate	4	[7]
O=N(=O)OCCCCCCCCC	1-octylnitrate	4	[9]
O=N(=O)OC(C)CCCCCC	2-octylnitrate	4	[7]
O=N(=O)OC(C)CCCCCC	2-octylnitrate	4	[9]
O=N(=O)OC(C)CCCCCC	2-octylnitrate	4	[11]
O=N(=O)OC(C)CCCCCC	2-octylnitrate	4	[11] (Kornblum)
O=N(=O)OCC(CC)CCCC	2-ethylhexylnitrate	4	[12]

SMILES	name	data type	reference
O=N(=O)OCCCCCCCCCC	1-decylnitrate	4	[6]
O=N(=O)OCCCCCCCCCCCC	1-dodecylnitrate	4	[6]
O=N(=O)OC1CCCC1	cyclopentylnitrate	1	[10]
O=N(=O)OC1CCCCC1	cyclohexylnitrate	1	[10]
monocarbonyls			
O=CC	ethanal	1	[2]
O=CCC	propanal	1	[2]
O=CCCC	butanal	1	[3]
O=CCCCC	pentanal	1	[2]
O=CCCCCC	hexanal	2	[13]
O=CCCCCC	hexanal	1	[2]
O=CCCCCCC	heptanal	1	[2]
O=CCCCCCCC	octanal	2	[13]
O=CCCCCCCC	octanal	1	[2]
O=CCCCCCCCC	nonanal	2	[13]
O=CCCCCCCCC	nonanal	1	[2]
O=CCCCCCCCCC	decanal	2	[13]
O=CCCCCCCCCC	decanal	1	[2]
O=CCCCCCCCCCC	undecanal	2	[13]
O=CCCCCCCCCCC	undecanal	1	[2]
O=CCCCCCCCCCCC	dodecanal	2	[13]
O=CCCCCCCCCCCC	dodecanal	1	[2]
O=CCCCCCCCCCCCC	tridecanal	2	[13]
O=CCCCCCCCCCCCC	tridecanal	1	[2]
O=CCCCCCCCCCCCCC	tetradecanal	2	[13]
O=CC(C)C	2-methylpropanal	1	[3]
O=CC(CC)CCCC	2-ethylhexanal	1	[2]

SMILES	name	data type	reference
O=CC=C	2-propenal	1	NIST (Stull)
O=CC=CC	2-butenal	1	[14]
O=CC=CC	trans-2-butenal	1	[3]
O=CC(C)=CC	2-methyl-2-butenal	1	[14]
O=CC(C)=C(C)C	2,3-dimethyl-2-butenal	1	[14]
O=CC=CC=CC	2,4-hexadienal	1	[14]
O=CCCCC=C	5-hexenal	1	[14]
CC(=O)C	propanone	1	[15]
CC(=O)CC	butanone	1	[15]
CC(=O)CCC	2-pentanone	1	[15]
CC(=O)CCCC	2-hexanone	1	[15]
CC(=O)CCCCC	2-heptanone	1	[15]
CC(=O)CCCCCC	2-octanone	1	[15]
CC(=O)CCCCCCC	2-nonanone	1	[15]
CC(=O)CCCCCCCC	2-decanone	1	[15]
CC(=O)CCCCCCCCC	2-undecanone	1	[15]
CC(=O)CCCCCCCCCC	2-dodecanone	1	[15]
CC(=O)CCCCCCCCCCC	2-tridecanone	1	[15]
CC(=O)CCCCCCCCCCCC	2-tetradecanone	1	[15]
CCC(=O)CC	3-pentanone	1	[15]
CCC(=O)CCC	3-hexanone	1	[15]
CCC(=O)CCCC	3-heptanone	1	[15]
CCCC(=O)CCC	4-heptanone	1	[15]
CCC(=O)CCCCC	3-octanone	2	[16]
CCCCC(=O)CCCC	5-nonanone	1	[15]
CCCCCC(=O)CCCCC	6-undecanone	1	[15]
CCCCCCC(=O)CCCCCC	7-tridecanone	1	[15]

SMILES	name	data type	reference
CC(=O)C(C)C	3-methyl-2-butanone	1	[15]
CC(=O)C(C)CC	3-methyl-2-pentanone	1	[15]
CC(=O)CC(C)C	4-methyl-2-pentanone	1	[15]
CC(=O)C(C)(C)C	3,3-dimethyl-2-butanone	1	[15]
CC(=O)C(C)CCC	3-methyl-2-hexanone	1	[15]
CC(=O)CC(C)CC	4-methyl-2-hexanone	1	[15]
CC(=O)CCC(C)C	5-methyl-2-hexanone	1	[15]
CC(=O)C(CC)CC	3-ethyl-2-pentanone	1	[15]
CC(=O)C(C)(C)CC	3,3-dimethyl-2-pentanone	1	[15]
CC(=O)C(C)C(C)C	3,4-dimethyl-2-pentanone	1	[15]
CC(=O)CC(C)(C)C	4,4-dimethyl-2-pentanone	1	[15]
CC(=O)C(C)CCCC	3-methyl-2-heptanone	3	NIST (Powell)
CC(C)C(=O)CC	2-methyl-3-pentanone	1	[15]
CC(C)C(=O)CCC	2-methyl-3-hexanone	1	[15]
CCC(=O)C(C)CC	4-methyl-3-hexanone	1	[15]
CCC(=O)CC(C)C	5-methyl-3-hexanone	1	[15]
CC(C)(C)C(=O)CC	2,2-dimethyl-3-pentanone	1	[15]
CC(C)C(=O)C(C)C	2,4-dimethyl-3-pentanone	1	[15]
CC(C)(C)C(=O)C(C)C	2,2,4-trimethyl-3-pentanone	1	NIST (Stull)
CC(C)CC(=O)CC(C)C	2,6-dimethyl-4-heptanone	1	[15]
CC(=O)C=C	3-buten-2-one	1	[14]
CC(=O)C=CC	3-penten-2-one	1	[14]
CC(=O)C(C)=C	3-methyl-3-butene-2-one	1	[2]
CC(=O)CCC=C	5-hexen-2-one	1	[14]
CC(=O)CCC=C	5-hexen-2-one	1	[17]
CCC(=O)CC=C	5-hexen-3-one	1	[14]
CC(=O)C(C)=CC	3-methyl-3-penten-2-one	1	[14]

SMILES	name	data type	reference
CC(=O)C=C(C)C	4-methyl-3-penten-2-one	1	[1]
CC(=O)CC(C)=C	4-methyl-4-penten-2-one	1	[14]
CC(=O)CCC(C)=C	5-methyl-5-hexen-2-one	1	[14]
O=C1CCC1	cyclobutanone	1	[15]
O=C1CCCC1	cyclopentanone	1	[15]
O=C1CCCCC1	cyclohexanone	1	[15]
O=C1CCCCCC1	cycloheptanone	1	[15]
O=C1C=CCCC1	2-cyclohexen-1-one	1	[18]
O=C1C=C(C)CC(C)(C)C1	3,5,5-trimethyl-2-cyclohexen-1-one	1	[2]
O=C1C(C)=CCC(C(C)=C)C1	2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	1	NIST (Stull)
O=C1C(C)=CCC(C(C)=C)C1	2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	2	[19]
O=CC(C)CC	2-methylbutanal	3	NIST (avg)
O=CCC(C)C	3-methylbutanal	3	NIST (avg)
O=CC(C)(C)C	2,2-dimethylpropanal	3	NIST (avg)
O=CC(C)CCC	2-methylpentanal	3	NIST (avg)
O=CCC(C)CC	3-methylpentanal	3	NIST (Levene)
O=CCCC(C)C	4-methylpentanal	3	NIST (avg)
O=CC(CC)CC	2-ethylbutanal	3	NIST (avg)
O=CC(C)(C)CC	2,2-dimethylbutanal	3	NIST (Kohlraush)
O=CCC(C)(C)C	3,3-dimethylbutanal	3	NIST (Pomerantz)
O=CC(C)CCCC	2-methylhexanal	3	[20]
O=CC1CCCCC1	cyclohexanecarboxaldehyde	3	NIST (Weast)
CCCC(=O)CCCC	4-octanone	3	NIST (avg)
CCC(=O)CCCCCC	3-nonanone	3	NIST (Aldrich)
CCCC(=O)CCCCC	4-nonanone	3	NIST (Weast)
CCC(=O)CCCCCCC	3-decanone	3	NIST (Aldrich)
CCCC(=O)CCCCCC	4-decanone	3	NIST (Weast)

SMILES	name	data type	reference
CCCCC(=O)CCCCC	5-decanone	3	NIST (Baykut)
O=C1C(C)CCCC1	2-methylcyclohexanone	3	NIST (White)
O=C1CC(C)CCC1	3-methylcyclohexanone	3	NIST (White)
O=C1CCC(C)CC1	4-methylcyclohexanone	3	NIST (Weast)
O=C1C(C)(C)CCCC1	2,2-dimethylcyclohexanone	3	[16]
O=C1C(C)C(C)CCC1	cis-2,3-dimethylcyclohexanone	3	[16]
O=C1C(C)CC(C)CC1	trans-2,4-dimethylcyclohexanone	3	[16]
O=C1C(C)CC(C)CC1	cis-2,4-dimethylcyclohexanone	3	[16]
O=C1C(C)CCC(C)C1	trans-2,5-dimethylcyclohexanone	3	[16]
O=C1C(C)CCCC1C	2,6-dimethylcyclohexanone	3	NIST (Weast)
O=C1CC(C)(C)CCC1	3,3-dimethylcyclohexanone	3	[16]
O=C1CC(C)C(C)CC1	3,4-dimethylcyclohexanone	3	NIST (VonAuwers)
O=C1CC(C)CC(C)C1	3,5-dimethylcyclohexanone	3	NIST (VonAuwers)
O=C1CCC(CC)CC1	4-ethylcyclohexanone	3	[16]
O=C1C(C)(CC)CCCC1	2-ethyl-2-methylcyclohexanone	3	[16]
O=C1C(C)CCC(C(C)=C)C1	2S-trans-2-methyl-5-(1-methylethenyl)-cyclohexanone	3	[16]
O=C1C(C)CCC(C(C)C)C1	2S-trans-2-methyl-5-(1-methylethyl)-cyclohexanone	3	[16]
O=C1C(C(C)C)CCC(C)C1	2R-cis-5-methyl-2-(1-methylethyl)-cyclohexanone	3	[16]
O=C1C(C(C)C)CCC(C)C1	2S-trans-5-methyl-2-(1-methylethyl)-cyclohexanone	3	[16]
O=C1C(C)CC(C)C1	2,4-dimethylcyclopentanone	3	NIST (Aldrich)
O=C1C=CCC1	2-cyclopenten-1-one	3	NIST (Weast)
O=C1CC=CCC1	3-cyclohexen-1-one	3	[16]
O=C1C(C)=CCC(C)C1	2,5-dimethyl-2-cyclohexenone	3	[16]
O=C1C=C(C)CC(C)C1	3,5-dimethyl-2-cyclohexenone	3	NIST (Aldrich)
O=C1C(C)=CCCC1	2-methyl-2-cyclohexenone	3	NIST (Weast)
O=C1C=C(C)CCC1	3-methyl-2-cyclohexenone	3	NIST (Weast)
O=C1C=CCC(C)C1	5-methyl-2-cyclohexenone	3	[16]

SMILES	name	data type	reference
O=C1CC(C)=CCC1	3-methyl-3-cyclohexenone	3	[16]
O=C1CC=C(C)CC1	4-methyl-3-cyclohexenone	3	[16]
O=C1C=C(C)CCC1(C(C)C)	piperitone	3	[16]
O=C1C=C(C(C)C)CCC1(C)	6-methyl-3-(1-methylethyl)-2-cyclohexen-1-one	3	[16]
O=C1C=C(C)C(C)(C)CC1	3,4,4-trimethyl-2-cyclohexen-1-one	3	NIST (Weast)
O=C1C=C(C)C(C)CC1(C)	3,4,6-trimethyl-2-cyclohexen-1-one	3	[16]
O=C1C=C(C)CCC1(C)(C)	3,6,6-trimethyl-2-cyclohexen-1-one	3	[16]
mono-ethers			
COC	1-methoxymethane	1	[15]
COCC	1-methoxyethane	1	[15]
COCCC	1-methoxypropane	1	[15]
COCCCC	1-methoxybutane	1	[15]
COCCCCC	1-methoxypentane	1	[15]
COCCCCCC	1-methoxyhexane	3	NIST (Majer)
COCCCCCCCC	1-methoxyoctane	3	NIST (Devaney)
COCCCCCCCCCC	1-methoxydecane	1	[15]
COC(C)C	2-methoxypropane	1	[15]
COC(C)CC	2-methoxybutane	1	[15]
COCC(C)C	1-methoxy-2-methylpropane	1	[15]
COC(C)(C)C	2-methoxy-2-methylpropane	1	[15]
COC(C)CCC	2-methoxypentane	1	[15]
COCC(C)CC	1-methoxy-2-methylbutane	1	[15]
COCCC(C)C	1-methoxy-3-methylbutane	1	[15]
COC(C)(C)CC	2-methoxy-2-methylbutane	1	[15]
COC(C)(C)CC	2-methoxy-2-methylbutane	2	[21]
COC(C)(C)CC(C)(C)C	2-methoxy-2	2	[21]
CCOCC	ethoxyethane	1	[15]

SMILES	name	data type	reference
CCOCCC	1-ethoxypropane	1	[15]
CCOCCCC	1-ethoxybutane	1	[15]
CCCOCCC	1-propoxypropane	1	[15]
CCOCCCCC	1-ethoxypentane	3	NIST (Weast)
CCCCOCCCC	1-butoxybutane	1	[15]
CCCOCCCCCCCC	1-propoxyoctane	3	NIST (Devaney)
CCOC(C)C	2-ethoxypropane	1	[15]
CCOC(C)CC	2-ethoxybutane	1	[15]
CCOCC(C)C	1-ethoxy-2-methylpropane	1	[15]
CCOC(C)(C)C	2-ethoxy-2-methylpropane	1	[15]
CCCOC(C)C	2-propoxypropane	1	[15]
CC(C)OC(C)C	diisopropylether	1	[15]
CCOC(C)(C)CC	2-ethoxy-2-methylbutane	2	[21]
CCOC(C)CCC	2-ethoxypentane	3	NIST (Frinton)
CCCOC(C)CC	s-butylpropylether	3	NIST (Majer)
CCCOCC(C)C	2-methyl-1-propoxypropane	3	NIST (Majer)
CCC(C)OC(C)CC	di-s-butylether	1	[15]
CC(C)COCC(C)C	diisobutylether	1	[15]
CC(C)COC(C)(C)C	t-butylisobutylether	2	[21]
CC(C)OCCCCC	isopropylpentylether	3	NIST (Majer)
CCCOC(C)(C)CC	2-propoxy-2-methylbutane	2	[21]
CC(C)(C)OC(C)(C)C	di-t-butylether	1	[15]
CCOC(C)(C)CC(C)(C)C	2-ethoxy-2,4,4-trimethylpentane	2	[21]
CCCCOC(C)(C)CC	butyl-t-pentylether	2	[21]
CCCOC(C)(C)CC(C)(C)C	2-propoxy-2,4,4-trimethylpentane	2	[21]
CCCCOC(C)(C)CC(C)(C)C	2-butoxy-2,4,4-trimethylpentane	2	[21]
CCC(C)(C)OC(C)(C)CC(C)(C)C	1,1-dimethylpropoxy-2,4,4-trimethylpentane	2	[21]

SMILES	name	data type	reference
CCCCCCOC(C)(C)CC(C)(C)C	hexoxy-2,4,4-trimethylpentane	2	[21]
C1OCC1	propyleneoxide	1	[15]
C1OCCC1	tetrahydrofuran	1	[15]
C1OCCCC1	tetrahydropyran	1	[3]
CC1OCCC1	2-methyltetrahydrofuran	1	[15]
C1OCC=C1	2,5-dihydrofuran	1	[3]
C1OC=CCC1	2,3-dihydro-4H-pyran	1	[3]
mono-esters			
CC(=O)OC	methylacetate	1	[2]
CC(=O)OCC	ethylacetate	1	[2]
CC(=O)OCCC	propylacetate	1	[2]
CC(=O)OCCCC	butylacetate	1	[2]
CC(=O)OCCCCC	pentylacetate	1	[2]
CC(=O)OCCCCCC	hexylacetate	1	[2]
CC(=O)OC(C)C	isopropylacetate	1	[2]
CC(=O)OC(C)CC	sec-butylacetate	1	[2]
CC(=O)OCC(C)C	isobutylacetate	1	[2]
CC(=O)OC(C)(C)C	t-butylacetate	1	[2]
CC(=O)OCCC(C)C	isopentylacetate	1	[2]
CCC(=O)OC	methylpropanoate	1	[2]
CCCC(=O)OC	methylbutanoate	1	[2]
CCC(=O)OCC	ethylpropanoate	1	[2]
CCCCC(=O)OC	methylpentanoate	1	[3]
CCCC(=O)OCC	ethylbutanoate	1	[2]
CCC(=O)OCCC	propylpropanoate	1	[2]
CCCCCC(=O)OC	methylhexanoate	1	[15]
CCCCC(=O)OCC	ethylpentanoate	1	[3]

SMILES	name	data type	reference
CCC(=O)OCCCC	butylpropanoate	1	[2]
CCCC(=O)OCCC	propylbutanoate	1	[2]
CCCC(=O)OCCCC	butylbutanoate	1	[3]
CCCCCC(=O)OCCC	propylhexanoate	1	[15]
CCCCCCCC(=O)OC	methyloctanoate	1	[15]
CCCCCCCC(=O)OCC	ethyloctanoate	1	[3]
CCCCCCCC(=O)OCCC	propyloctanoate	1	[15]
CCC(=O)OCCCCCCCC	octylacrylate	3	NIST (Bilterys)
CCCCCCCCCC(=O)OC	methyldecanoate	1	[15]
CCCCCCCCCC(=O)OCCC	propyldecanoate	1	[15]
CCCCCCCCCCCC(=O)OC	methyldodecanoate	1	[15]
CC(C)C(=O)OC	methylisobutanoate	1	[3]
CC(C)C(=O)OCC	ethylisobutanoate	1	[3]
CCC(=O)OCC(C)C	isobutylpropanoate	1	[3]
CCCC(=O)OCC(C)C	isobutylbutanoate	1	[3]
CC(C)C(=O)OCC(C)C	isobutylisobutanoate	1	[2]
CC(C)CC(=O)OC	methylisovalerate	1	[15]
CC(C)CC(=O)OCC	ethylisovalerate	1	[15]
CC(C)CC(=O)OCCC	propylisovalerate	1	[15]
CC(C)CC(=O)OC(C)C	isopropylisovalerate	1	[15]
CC(C)CC(=O)OCC(C)C	isobutylisovalerate	1	[15]
CC(C)CC(=O)OCCC(C)C	isopentylisovalerate	1	[15]
C=CC(=O)OC	methylacrylate	1	[15]
C=CC(=O)OCC	ethylacrylate	1	[15]
C=CC(=O)OCCC	propylacrylate	1	[2]
C=CC(=O)OCCCC	butylacrylate	1	[15]
C=CC(=O)OCC(C)C	isobutylacrylate	1	[15]

SMILES	name	data type	reference
CC(=O)OC=C	vinylacetate	1	[2]
C=C(C)C(=O)OC	methylmethacrylate	1	[15]
C=C(C)C(=O)OCC	ethylmethacrylate	1	[15]
C=C(C)C(=O)OCCCC	butylmethacrylate	1	[15]
C=C(C)C(=O)OCC(C)C	isobutylmethacrylate	1	[15]
C=CC(=O)OCCCCCCCC	octylacrylate	1	[15]
C=CC(=O)OCC(CC)CCCC	2-ethylhexylacrylate	1	[15]
monoperoxides			
COOC	dimethylperoxide	4	[22]
COOCC	ethylmethylperoxide	3	[23]
COOC(C)C	isopropylmethylperoxide	3	[23]
CCOOCC	diethylperoxide	1	[24]
COOC(C)(C)C	t-butylmethylperoxide	4	[22]
CC(C)(C)OOC(C)(C)C	di-t-butylperoxide	1	[24]
CC(C)(C)OOC(C)(C)C	di-t-butylperoxide	1	[25]
CC(C)(C)OOC(C)(C)C	di-t-butylperoxide	1	[2]
CC(C)(C)OOC(C)(C)CC	t-butyl-t-pentylperoxide	3	[23]
CCC(C)(C)OOC(C)(C)CC	di-t-pentylperoxide	4	[22]
C1COOCC1	1,2-dioxane	4	[22]
C1(C)(C)OOC(C)(C)C1	3,3,5,5-tetramethyl-1,2-dioxolane	4	[22]
C1C(C)(C)OOC(C)(C)C1	3,3,6,6-tetramethyl-1,2-dioxane	4	[22]
monoperoxy acyl nitrates			
O=N(=O)OOC(=O)C	peroxyacetylnitrate	1	[26]
O=N(=O)OOC(=O)C	peroxyacetylnitrate	2	[27]
O=N(=O)OOC(=O)CC	peroxypropionylnitrate	9	[28]
O=N(=O)OOC(=O)CCC	peroxybutylnitrate	9	[28]
O=N(=O)OOC(=O)C(C)C	peroxyisobutylnitrate	9	[28]

SMILES	name	data type	reference
O=N(=O)OOC(=O)C(=C)C	peroxy-2-propenoylnitrate	9	[28]
mono-alcohols			
OCC	ethanol	1	[15]
OCCC	1-propanol	1	[15]
OCCCC	1-butanol	1	[15]
OCCCCC	1-pentanol	1	[15]
OCCCCCC	1-hexanol	1	[15]
OCCCCCC	1-hexanol	2	[29]
OCCCCCCC	1-heptanol	1	[15]
OCCCCCCCC	1-octanol	1	[15]
OCCCCCCCC	1-octanol	2	[29]
OCCCCCCCCC	1-nonanol	1	[15]
OCCCCCCCCCC	1-decanol	1	[15]
OCCCCCCCCCC	1-decanol	2	[29]
OCCCCCCCCCCC	1-undecanol	1	[15]
OCCCCCCCCCCC	1-undecanol	2	[29]
OCCCCCCCCCCCC	1-dodecanol	1	[15]
OCCCCCCCCCCCC	1-dodecanol	2	[29]
OCCCCCCCCCCCCC	1-tridecanol	1	[15]
OCCCCCCCCCCCCC	1-tridecanol	2	[29]
OCCCCCCCCCCCCCC	1-tetradecanol	1	[15]
OCCCCCCCCCCCCCC	1-tetradecanol	2	[29]
OCC=C	2-propen-1-ol	1	[3]
OCCC=C	3-buten-1-ol	1	[14]
OCC=CCC	2-penten-1-ol	1	[14]
OCCC=CC	3-penten-1-ol	1	[14]
OCC(C)C	2-methyl-1-propanol	1	[15]

SMILES	name	data type	reference
OCC(C)CC	2-methyl-1-butanol	1	[15]
OCCC(C)C	3-methyl-1-butanol	1	[15]
OCC(C)(C)C	2,2-dimethyl-1-propanol	1	[15]
OCC(C)(C)C	2,2-dimethyl-1-propanol	2	[30]
OCC(C)CCC	2-methyl-1-pentanol	1	[15]
OCC(C)CCC	2-methyl-1-pentanol	2	[30]
OCCC(C)CC	3-methyl-1-pentanol	1	[15]
OCCC(C)CC	3-methyl-1-pentanol	2	[30]
OCCCC(C)C	4-methyl-1-pentanol	1	[15]
OCC(CC)CC	2-ethyl-1-butanol	1	[15]
OCC(CC)CC	2-ethyl-1-butanol	2	[30]
OCC(C)(C)CC	2,2-dimethyl-1-butanol	1	[15]
OCC(C)C(C)C	2,3-dimethyl-1-butanol	1	[15]
OCCC(C)(C)C	3,3-dimethyl-1-butanol	1	[15]
OCCC(C)(C)C	3,3-dimethyl-1-butanol	2	[30]
OCC(C)CCCC	2-methyl-1-hexanol	1	[3]
OCCCCC(C)C	5-methyl-1-hexanol	1	[2]
OCC(CC)CCCC	2-ethyl-1-hexanol	1	[15]
OCC(CC)CC(C)C	4-methyl-2-ethyl-1-pentanol	1	[15]
OCCCCCCCC(C)C	8-methyl-1-nonanol	1	[2]
OCC(C)=CC	2-methyl-2-buten-1-ol	1	[14]
OCCC(C)=C	3-methyl-3-buten-1-ol	1	[14]
OCCC=C(C)C	4-methyl-3-penten-1-ol	1	[14]
OCC(C)=C(C)C	2,3-dimethyl-2-buten-1-ol	1	[14]
OCC=C(C)CCC=C(C)C	3,7-dimethyl-trans-2,6-octadien-1-ol	2	[16]
CC(O)C	2-propanol	1	[15]
CC(O)CC	2-butanol	1	[15]

SMILES	name	data type	reference
CC(O)CCC	2-pentanol	1	[15]
CC(O)CCCC	2-hexanol	2	[31]
CC(O)CCCC	2-hexanol	2	[30]
CC(O)CCCCC	2-heptanol	2	[31]
CC(O)CCCCC	2-heptanol	2	[32]
CC(O)CCCCCC	2-octanol	2	[31]
CC(O)CCCCCC	2-octanol	2	[32]
CC(O)CCCCCCC	2-nonanol	2	[31]
CC(O)CCCCCCC	2-nonanol	2	[32]
CC(O)CCCCCCCC	2-decanol	2	[31]
CC(O)CCCCCCCCC	2-undecanol	2	[31]
CC(O)CCCCCCCCCC	2-dodecanol	2	[31]
CC(O)CCCCCCCCCCC	2-tetradecanol	2	[31]
CCC(O)CC	3-pentanol	1	[15]
CCC(O)CCC	3-hexanol	2	[31]
CCC(O)CCC	3-hexanol	2	[30]
CCC(O)CCCC	3-heptanol	2	[31]
CCCC(O)CCC	4-heptanol	2	[32]
CCC(O)CCCCC	3-octanol	2	[31]
CCC(O)CCCCC	3-octanol	2	[32]
CCCC(O)CCCC	4-octanol	2	[32]
CCC(O)CCCCCC	3-nonanol	2	[31]
CCC(O)CCCCCC	3-nonanol	2	[32]
CCCC(O)CCCCC	4-nonanol	2	[32]
CCCCC(O)CCCC	5-nonanol	2	[32]
CC(O)C(C)C	3-methyl-2-butanol	1	[15]
CC(O)C(C)C	3-methyl-2-butanol	2	[30]

SMILES	name	data type	reference
CC(O)C(C)CC	3-methyl-2-pentanol	1	[15]
CC(O)C(C)CC	3-methyl-2-pentanol	2	[30]
CC(O)CC(C)C	4-methyl-2-pentanol	1	[15]
CC(O)CC(C)C	4-methyl-2-pentanol	2	[30]
CC(O)C(C)(C)C	3,3-dimethyl-2-butanol	1	[15]
CC(O)C(C)(C)C	3,3-dimethyl-2-butanol	2	[30]
CC(C)C(O)CC	2-methyl-3-pentanol	1	[15]
CC(C)C(O)CC	2-methyl-3-pentanol	2	[30]
CC(C)(C)C(O)CC	2,2-dimethyl-3-pentanol	2	[16]
CC(C)C(O)C(C)C	2,4-dimethyl-3-pentanol	1	[15]
CC(C)CC(O)CC(C)C	2,6-dimethyl-4-heptanol	1	[15]
CC(O)C=C	3-buten-2-ol	1	[14]
CC(O)C(C)=CC	3-methyl-3-penten-2-ol	1	[14]
CC(O)CC(C)=C	4-methyl-4-penten-2-ol	1	[14]
C=C(C)C(O)CC	2-methyl-1-penten-3-ol	1	[14]
CC(O)(C)C	2-methyl-2-propanol	1	[15]
CC(O)(C)CC	2-methyl-2-butanol	1	[15]
CC(O)(C)CC	2-methyl-2-butanol	2	[30]
CC(O)(C)CCC	2-methyl-2-pentanol	1	[15]
CCC(O)(C)CC	3-methyl-3-pentanol	1	[15]
CCC(O)(C)CC	3-methyl-3-pentanol	2	[30]
CC(O)(C)C(C)C	2,3-dimethyl-2-butanol	1	[15]
CC(O)(C)CCCC	2-methyl-2-hexanol	1	[15]
CCC(O)(C)CCC	3-methyl-3-hexanol	3	NIST (avg)
CC(O)(CC)CCCC	3-methyl-3-heptanol	2	[16]
CCCC(O)(C)CCC	4-methyl-4-heptanol	2	[16]
CC(O)(C)CC(C)(C)C	2,4,4-trimethyl-2-pentanol	2	[16]

SMILES	name	data type	reference
CC(O)(C)CC=C	2-methyl-4-penten-2-ol	1	[14]
OC1CCC1	cyclobutanol	1	[33]
OC1CCCC1	cyclopentanol	1	[15]
OC1CCCCC1	cyclohexanol	1	[15]
OC1CCCCCC1	cycloheptanol	3	NIST (Weast)
OC1CCCCCC1	cycloheptanol	1	[3]
OC1(C)CCCCC1	1-methylcyclohexanol	1	[2]
OC1C(C)CCCC1	cis-2-methylcyclohexanol	1	[2]
OC1C(C)CCCC1	trans-2-methylcyclohexanol	1	[2]
OC1C(C)CCCC1	2-methylcyclohexanol	1	[34]
OC1CC(C)CCC1	cis-3-methylcyclohexanol	1	[2]
OC1CC(C)CCC1	trans-3-methylcyclohexanol	1	[2]
OC1CCC(C)CC1	cis-4-methylcyclohexanol	1	[2]
OC1CCC(C)CC1	trans-4-methylcyclohexanol	1	[2]
OC1C(C)CC(C)C1	2,4-dimethylcyclopentanol	1	[33]
CCCC(O)CCCCCC	4-decanol	3	NIST (Weast)
OCC1CCCCC1	cyclohexylmethanol	3	NIST (Weast)
CC(O)C(C)CCC	3-methyl-2-hexanol	3	NIST (avg)
CC(O)CC(C)CC	4-methyl-2-hexanol	3	NIST (avg)
CC(C)C(O)CCC	2-methyl-3-hexanol	3	NIST (avg)
CCC(O)C(C)CC	4-methyl-3-hexanol	3	NIST (avg)
CCC(O)CC(C)C	5-methyl-3-hexanol	3	NIST (Benkeser)
OC1C(C)(C)CCCC1	2,2-dimethylcyclohexanol	3	[16]
OC1C(C)CC(C)CC1	2,4-dimethylcyclohexanol	3	[16]
OC1C(C)CCCC1(C)	2,6-dimethylcyclohexanol	3	[16]
OC1CC(C)(C)CCC1	3,3-dimethylcyclohexanol	3	[16]
OC1CC(C)C(C)CC1	3,4-dimethylcyclohexanol	3	[16]

SMILES	name	data type	reference
OC1CC(C)CC(C)C1	3,5-dimethylcyclohexanol	3	[16]
OC1CCC(C)(C)CC1	4,4-dimethylcyclohexanol	3	[16]
OC1C(CC)CCCC1	cis-2-ethylcyclohexanol	3	[16]
OC1(CC)CCCCC1	1-ethylcyclohexanol	3	NIST (Weast)
OC1(C)C(C)CCCC1	1,2-dimethylcyclohexanol	3	NIST (VonAuwers)
OC1(C)CC(C)CCC1	1,3-dimethylcyclohexanol	3	NIST (Sabatier)
OC1(C)CCC(C)CC1	1,4-dimethylcyclohexanol	3	NIST (Sabatier)
OC1(CCC)CCCC1	1-propylcyclopentanol	3	NIST (Weast)
OC1(CCC)CCCCC1	1-propylcyclohexanol	3	NIST (Nenitzescu)
OC1(CC)C(C)CCCC1	1-ethyl-2-methylcyclohexanol	3	[16]
OC1(CCC)CC(C)CCC1	3-methyl-1-propylcyclohexanol	3	[16]
OC1C(C)C(C2)C(C)(C)C2C1	(1R,2R,3R,5S)-(-)-isopinocampheol	3	[35]
OCC1C(C2)C(C)(C)C2CC1	trans-myrtanol	2	[19]
OCC1C(C2)C(C)(C)C2CC1	trans-myrtanol	3	[35]
OC1C(=C)C(C2)C(C)(C)C2C1	trans-pinocarveol	2	[19]
mono-acids			
OC(=O)C	ethanoicacid	5	[15, 36]
OC(=O)CC	propanoicacid	5	[15, 36]
OC(=O)CCC	butanoicacid	5	[15, 36]
OC(=O)CCCC	pentanoicacid	5	[15, 36]
OC(=O)CCCCC	hexanoicacid	1	[15]
OC(=O)CCCCCC	heptanoicacid	1	[15]
OC(=O)CCCCCCC	octanoicacid	1	[15]
OC(=O)CCCCCCCC	nonanoicacid	1	[15]
OC(=O)CCCCCCCCC	decanoicacid	1	[15]
OC(=O)C(C)C	2-methylpropanoicacid	5	[15, 36]
OC(=O)C1CC1	cyclopropanoicacid	1	[17]

SMILES	name	data type	reference
OC(=O)C(C)CC	2-methylbutanoicacid	1	[2]
OC(=O)CC(C)C	3-methylbutanoicacid	1	[15]
OC(=O)C(C)(C)C	trimethylaceticacid	1	[37]
OC(=O)C1CCC1	cyclobutanoicacid	1	[33]
OC(=O)C(C)CCC	2-methylpentanoicacid	3	NIST (avg)
OC(=O)CC(C)CC	3-methylpentanoicacid	3	NIST (avg)
OC(=O)CCC(C)C	4-methylpentanoicacid	1	[15]
OC(=O)C(CC)CC	2-ethylbutanoicacid	3	NIST (avg)
OC(=O)C(CC)CC	2-ethylbutanoicacid	4	NIST (Aldrich)
OC(=O)C(CC)CC	2-ethylbutanoicacid	4	NIST (Weast)
OC(=O)C1CCCC1	cyclopentanecarboxylicacid	3	NIST (Aldrich)
OC(=O)C1CCCC1	cyclopentanecarboxylicacid	4	NIST (Weast)
OC(=O)C1CCCC1	cyclopentanecarboxylicacid	4	NIST (Frinton)
OC(=O)C1CCCCC1	cyclohexanecarboxylicacid	3	NIST (Weast)
OC(=O)C1CCCCC1	cyclohexanecarboxylicacid	4	NIST (Weast)
OC(=O)CC1CCCC1	cyclopentaneaceticacid	3	NIST (Weast)
OC(=O)CC1CCCC1	cyclopentaneaceticacid	4	NIST (Aldrich)
OC(=O)CC1CCCCC1	cyclohexaneaceticacid	3	NIST (Weast)
OC(=O)CC1CCCCC1	cyclohexaneaceticacid	4	NIST (Weast)
OC(=O)CCC1CCCC1	cyclopentanepropanoicacid	4	NIST (Weast)
OC(=O)CCC1CCCCC1	cyclohexanepropanoicacid	3	NIST (Weast)
OC(=O)C=C	propenoicacid	1	[15]
OC(=O)C(C)=C	2-methylpropenoicacid	1	[15]
OC(=O)C=CC	cis-2-butenoicacid	1	[15]
OC(=O)C=CC	trans-2-butenoicacid	1	[15]
OC(=O)C(C)=CC	cis-2-methyl-2-butenoicacid	1	[15]
OC(=O)C(C)=CC	trans-2-methyl-2-butenoicacid	1	[15]

SMILES	name	data type	reference
OC(=O)C=C(C)C	3-methyl-2-butenoicacid	3	NIST (Weast)
OC(=O)C=CCCC	trans-2-hexenoicacid	3	NIST (Aldrich)
OC(=O)C=CC=CC	trans,trans-2,4-hexadienoicacid	4	[16]
OC(=O)C(C)=CCC	2-methylpentenoicacid	3	[16]
OC(=O)C(C)=CCC	2-methylpentenoicacid	4	[16]
OC(=O)C=CC(C)C	4-methyl-2-pentenoicacid	3	[16]
OC(=O)C=CCCCC	2-heptenoicacid	3	NIST (Weast)
OC(=O)C=CCCCCC	2-octenoicacid	3	NIST (vanRomburgh)
OC(=O)CC=C	3-butenoicacid	1	[33]
OC(=O)CC=CC	3-pentenoicacid	3	[35]
OC(=O)CC=CC	3-pentenoicacid	4	NIST (Frinton)
OC(=O)CCC=C	4-pentenoicacid	3	NIST (Weast)
OC(=O)CCC=C	4-pentenoicacid	4	NIST (Aldrich)
OC(=O)CC=CCC	3-hexenoicacid	3	NIST (Weast)
OC(=O)CCCC=C	5-hexenoicacid	3	NIST (Lide)
OC(=O)C(C)C=CC	2-methyl-3-pentenoicacid	3	[16]
OC(=O)C(C)C=CC	2-methyl-3-pentenoicacid	4	[38]
OC(=O)C(C)(C)C=C	2,2-dimethyl-3-butenoicacid	3	NIST (Weast)
OC(=O)C(C)(C)C=C	2,2-dimethyl-3-butenoicacid	4	NIST (Weast)
OC(=O)CCCCCC=C	6-heptenoicacid	3	NIST (Weast)
OC(=O)CCCCCC=C	6-heptenoicacid	4	NIST (Weast)
OC(=O)CCC=C(C)C	5-methyl-4-hexenoicacid	3	[16]
OC(=O)CC(C)(C)CC(C)C	3,3,5-trimethyl-5-hexenoicacid	3	NIST (Eykman)
OC(=O)CC(C)CCC=C(C)C	3,7-dimethyl-6-octenoicacid	1	NIST (Stull)
monohydroperoxides			
OOC	hydroperoxymethane	1	[24]
OOCC	hydroperoxyethane	1	[24]

SMILES	name	data type	reference
OOC(C)(C)C	2-hydroperoxy-2-methyl-propane	1	[24]
OOC(C)(C)C	2-hydroperoxy-2-methyl-propane	1	[2]
OOC1CCCCC1	hydroperoxycyclohexane	4	[22]
monoperacids			
OOC(=O)C	aceticperoxyacid	1	[24]
OOC(=O)CC	propanoicperoxyacid	1	[24]
OOC(=O)CCC	butanoicperoxyacid	1	[24]
OOC(=O)CCCCC	hexanoicperoxyacid	4	[22]
bifunctional			
dinitrates			
O=N(=O)OCCON(=O)=O	1,2-ethylenedinitrate	2	[39]
O=N(=O)OCC(C)ON(=O)=O	1,2-propylenedinitrate	2	[39]
O=N(=O)OCCCON(=O)=O	1,3propylenedinitrate	2	[39]
O=N(=O)OCCCON(=O)=O	1,3propylenedinitrate	2	[40]
O=N(=O)OCCCCON(=O)=O	1,4-dinitroxybutane	2	[40]
O=N(=O)OCCC(C)ON(=O)=O	1,3-dinitroxybutane	2	[40]
O=N(=O)OCCCCCON(=O)=O	1,5-dinitroxypentane	2	[40]
O=N(=O)OC(C)CC(C)ON(=O)=O	2,4-dinitroxypentane	2	[40]
O=N(=O)OC(C)CCCC(C)ON(=O)=O	2,5-dinitroxyhexane	2	[40]
O=N(=O)OC1C(ON(=O)=O)CCCC1	cis-1,2-cyclohexyldinitrate	4	[11]
O=N(=O)OC1C(ON(=O)=O)CCCC1	trans-1,2-cyclohexyldinitrate	4	[11]
dicarbonyls			
CC(=O)C(=O)C	2,3-butadione	3	NIST (Weast)
CC(=O)C(=O)C	2,3-butadione	1	NIST
CC(=O)CC(=O)C	2,4-pentadione	3	NIST (avg)
CC(=O)CC(=O)C	2,4-pentadione	1	[3]
CC(=O)CC(=O)CC	2,4-hexadione	3	NIST (Weast)

SMILES	name	data type	reference
CC(=O)CC(=O)CC	2,4-hexadione	1	[33]
O=C1C(C(=O)C)CCC1	2-acetyl-cyclopentanone	3	[33]
O=C1C(C(=O)C)CCC1	2-acetyl-cyclopentanone	1	[33]
CC(=O)C(=O)CC	2,3-pentadione	3	NIST (Weast)
CC(=O)C(=O)CCC	2,3-hexadione	3	NIST (Weast)
CC(=O)CCC(=O)C	2,5-hexadione	3	NIST (Sabatier)
CCC(=O)C(=O)CC	3,4-hexadione	3	NIST (Weast)
CC(=O)CC(=O)CCC	2,4-heptadione	3	NIST (Weast)
CC(=O)CCCC(=O)C	2,6-heptadione	3	[16]
CC(=O)C(=O)C(C)C	4-methyl-2,3-pentadione	3	[38]
CC(=O)C(C)C(=O)C	3-methyl-2,4-pentadione	3	NIST (Sabatier)
CC(=O)C(=O)CC(C)C	5-methyl-2,3-hexadione	3	[38]
O=CC=O	glyoxal	3	NIST (Weast)
O=CC(=O)C	methylglyoxal	3	NIST (Weast)
O=CC(=O)CCC	2-oxopentanal	3	NIST (Weast)
CC(=O)CC1C(C)(C)C1CC(=O)	caronaldehyde	1	[41]
CC(=O)C1CC(C1(C)C)CC=O	pinonaldehyde	1	[41]
diols			
OCCO	1,2-ethanediol	1	[15]
OCCO	1,2-ethanediol	2	[42]
OCCCO	1,3-propanediol	1	[15]
OCCCO	1,3-propanediol	2	[43]
OCCCCO	1,4-butanediol	1	[15]
OCCCCCO	1,5-pentanediol	1	[15]
OCCCCCCO	1,6-hexanediol	1	[15]
OCCCCCCO	1,6-hexanediol	1	[44]
OCCCCCCO	1,6-hexanediol	2	[45]

SMILES	name	data type	reference
OCCCCCCCO	1,7-heptanediol	1	[46]
OCCCCCCCCO	1,8-octanediol	1	[44]
OCCCCCCCCCO	1,9-nonanediol	1	[46]
OCCCCCCCCCCO	1,10-decanediol	1	[44]
OCC(C)CO	2-methylpropane-1,3-diol	1	[15]
OCC(C)CO	2-methylpropane-1,3-diol	2	[43]
OCC(C)(C)CO	2,2-dimethylpropane-1,3-diol	7	[43, 43, 43]
OCCC(C)CCO	3-methyl-1,5-pentanediol	3	[47]
OCCC(C)CCO	3-methyl-1,5-pentanediol	2	[47]
OCC(CCCC)(CC)CO	2-butyl-2-ethyl-1,3-propanediol	1	[48]
OCC=CCO	2-butene-1,4-diol	1	[15]
CC(O)C(O)C	2,3-butanediol	1	[15]
CC(O)CC(O)C	2,4-pentanediol	3	[15]
CC(O)CC(O)C	2,4-pentanediol	2	[43]
CC(O)C(O)CC	2,3-pentanediol	3	[33]
CC(O)C(O)CC	2,3-pentanediol	1	[33]
CC(O)CCC(O)C	2,5-hexanediol	1	[15]
CC(O)(C)C(O)(C)C	2,3-dimethyl-2,3-butanediol	1	[15]
OCC(O)C	1,2-propanediol	1	[15]
OCC(O)C	1,2-propanediol	2	[42]
OCC(O)CC	1,2-butanediol	3	[15]
OCC(O)CC	1,2-butanediol	1	[15]
OCC(O)CC	1,2-butanediol	2	[42]
OCCC(O)C	1,3-butanediol	1	[15]
OCCC(O)C	1,3-butanediol	2	[43]
OCC(O)(C)C	2-methylpropane-1,2-diol	1	[15]
OCC(O)CCC	1,2-pentanediol	1	[15]

SMILES	name	data type	reference
OCC(O)CCC	1,2-pentanediol	2	[42]
OCCCC(O)C	1,4-pentanediol	1	[15]
OCC(O)CCCC	1,2-hexanediol	1	[15]
OCC(O)CCCC	1,2-hexanediol	2	[42]
CC(O)(C)CC(O)C	2-methylpentane-2,4-diol	1	[15]
CC(O)(C)CC(O)C	2-methylpentane-2,4-diol	2	[43]
OCC(O)CCCCCC	1,2-octanediol	2	[42]
OCC(C)(C)C(O)C(C)C	2,2,4-trimethyl-1,3-pentanediol	1	[48]
OC1C(O)CCCC1	1,2-cyclohexanediol	1	[15]
OC1CC(O)CCC1	1,3-cyclohexanediol	1	[15]
OC1CCC(O)CC1	1,4-cyclohexanediol	1	[15]
diacids			
OC(=O)C(=O)O	ethanoicdiacid	1	[2]
OC(=O)C(=O)O	ethanoicdiacid	1	[49]
OC(=O)C(=O)O	ethanoicdiacid	6	[49, 50, 51]
OC(=O)CC(=O)O	propanoicdiacid	1	[49]
OC(=O)CC(=O)O	propanoicdiacid	1	[52]
OC(=O)CC(=O)O	propanoicdiacid	6	[49, 53, 53]
OC(=O)CC(=O)O	propanoicdiacid	1	[54]
OC(=O)CCC(=O)O	butanoicdiacid	1	[3]
OC(=O)CCC(=O)O	butanoicdiacid	1	[49]
OC(=O)CCC(=O)O	butanoicdiacid	1	[54]
OC(=O)CCC(=O)O	butanoicdiacid	6	[49, 53, 53]
OC(=O)CCC(=O)O	butanoicdiacid	6	[55, 53, 53]
OC(=O)CCCC(=O)O	pentanoicdiacid	1	[15]
OC(=O)CCCC(=O)O	pentanoicdiacid	1	[49]
OC(=O)CCCC(=O)O	pentanoicdiacid	1	[54]

SMILES	name	data type	reference
OC(=O)CCCC(=O)O	pentanoicdiacid	1	[52]
OC(=O)CCCC(=O)O	pentanoicdiacid	6	[49, 53, 53]
OC(=O)CCCC(=O)O	pentanoicdiacid	6	[55, 53, 53]
OC(=O)CCCCC(=O)O	hexanoicdiacid	1	[15]
OC(=O)CCCCC(=O)O	hexanoicdiacid	1	[54]
OC(=O)CCCCC(=O)O	hexanoicdiacid	6	[55, 53, 53]
OC(=O)CCCCCC(=O)O	heptanoicdiacid	1	[15]
OC(=O)CCCCCC(=O)O	heptanoicdiacid	6	[55, 56, 56]
OC(=O)CCCCCCC(=O)O	octanoicdiacid	1	[15]
OC(=O)CCCCCCC(=O)O	octanoicdiacid	6	[55, 56, 56]
OC(=O)CCCCCCCC(=O)O	nonanoicdiacid	1	[15]
OC(=O)CCCCCCCC(=O)O	nonanoicdiacid	6	[55, 56, 56]
OC(=O)CCCCCCCCC(=O)O	decanoicdiacid	1	[15]
OC(=O)CCCCCCCCC(=O)O	decanoicdiacid	6	[55, 56, 56]
OC(=O)C(C)C(=O)O	methylpropanoicdiacid	8	[57]
OC(=O)C(C)C(=O)O	methylpropanoicdiacid	6	[53]
OC(=O)C(C)CC(=O)O	2-methylbutanoicdiacid	8	[57]
OC(=O)C(C)CC(=O)O	2-methylbutanoicdiacid	6	[58, 53, 53]
OC(=O)C(C)CC(=O)O	2-methylbutanoicdiacid	6	[53]
OC(=O)C(CC)C(=O)O	ethylpropanoicacid	6	[59, 59, 51]
OC(=O)C(C)(C)C(=O)O	dimethylpropanoicdiacid	8	[57]
OC(=O)C(C)(C)C(=O)O	dimethylpropanoicdiacid	6	[59, 59, 51]
OC(=O)C(C)CCC(=O)O	2-methylpentanoicdiacid	6	[58, 53, 53]
OC(=O)C(C)CCC(=O)O	2-methylpentanoicdiacid	6	[53, 53, 53]
OC(=O)CC(C)CC(=O)O	3-methylpentanoicdiacid	8	[57]
OC(=O)CC(C)CC(=O)O	3-methylpentanoicdiacid	6	[53, 53, 53]
OC(=O)C(C)(C)CC(=O)O	2,2-dimethylbutanoicdiacid	8	[57]

SMILES	name	data type	reference
OC(=O)C(C)(C)CC(=O)O	2,2-dimethylbutanoicdiacid	6	[58, 57, 51]
OC(=O)CC(C)CCC(=O)O	3-methyladipicacid	8	[57]
OC(=O)C(CCCC)C(=O)O	butylmalonicacid	6	[59, 59, 51]
OC(=O)C(C)(C)CCC(=O)O	2,2-dimethylpentanoicdiacid	6	[58, 58, 51]
OC(=O)CC(C)(C)CC(=O)O	3,3-dimethylpentanoicdiacid	8	[57]
CC1(C(CC1C(=O)O)CC(=O)O)C	pinicacid	8	[60, 60, 51]
CC1(C(CC1C(=O)O)CC(=O)O)C	pinicacid	8	[61, 60, 51]
O=C(O)C1(C(=O)O)CC1	1,1-cyclopropanedicarboxylicacid	7	[62, 62, 62]
O=C(O)C1(C(=O)O)CCC1	1,1-cyclobutanedicarboxylicacid	7	[62, 62, 62]
O=C(O)C1C(C(=O)O)CCC1	1,2-cyclopentanedicarboxylicacid	7	[62, 62, 62]
O=C(O)C1CC(C(=O)O)CCC1	1,3-cyclohexanedicarboxylicacid	7	[62, 62, 62]
O=C(O)C1CC(C(=O)O)C1(C)C	norpinicacid	8	[60, 60, 51]
OC(=O)C=CC(=O)O	trans-butenedioicacid	1	[3]
OC(=O)C=CC(=O)O	cis-butenedioicacid	1	[3]
OC(=O)C(C)=CC(=O)O	2-methyl-2-butenoicdiacid	1	[2]
OC(=O)C(=C)CC(=O)O	2-methylene-butanoicdiacid	1	[2]
OC(=O)C1CC(C(=O)O)CC1	1,4-cyclohexanedicarboxylicacid	1	[2]
diethers			
COCOC	dimethoxymethane	3	NIST (avg)
COCOC	dimethoxymethane	1	NIST (Nicolini)
COCCOC	1,2-dimethoxyethane	3	NIST (avg)
COCCOC	1,2-dimethoxyethane	1	[2]
CCOCOCC	diethoxymethane	3	NIST (avg)
CCOCOCC	diethoxymethane	1	NIST (Nicolini)
CCOCCOCC	1,2-diethoxyethane	3	NIST (avg)
CCOCCOCC	1,2-diethoxyethane	1	NIST (Stull)
CCOCCOCC	1,2-diethoxyethane	1	[63]

SMILES	name	data type	reference
CCOCCCOCC	1,3-diethoxypropane	3	NIST (Majer)
CCCCOCCOCCCC	1,2-dibutoxyethane	3	NIST (Kusano)
COC(C)OC	1,1-dimethoxyethane	3	NIST (Weast)
COC(C)OC	1,1-dimethoxyethane	1	NIST (Nicolini)
CCOC(C)OCC	1,1-diethoxyethane	3	NIST (Weast)
CCOC(C)OCC	1,1-diethoxyethane	1	NIST (Nicolini)
COC(C)(C)OC	2,2-dimethoxypropane	3	NIST (Weast)
CCOC(C(C)C)OCC	1,1-diethoxy-2-methylpropane	3	NIST (Adams)
CCOC(CC)OCC	1,1-diethoxypropane	3	NIST (Aldrich)
CCOC(CCC)OCC	1,1-diethoxybutane	3	NIST (Weast)
CCOC(C)(C)OCC	2,2-diethoxypropane	3	NIST (ATK)
C1OCCOC1	1,4-dioxane	1	[15]
C1OCOCC1	1,3-dioxane	1	NIST (Aldrich)
C1OCOC(C)(C)C1	4,4-dimethyl-1,3-dioxane	1	NIST (Lesteva)
diesters			
COC(=O)C(=O)OC	dimethyloxalate	3	[15]
COC(=O)C(=O)OC	dimethyloxalate	1	[15]
COC(=O)C(=O)OCC	methylethyloxalate	1	[15]
CCOC(=O)C(=O)OCC	diethyloxalate	1	[15]
CCCOC(=O)C(=O)OCCC	dipropyloxalate	1	[15]
CC(C)OC(=O)C(=O)OC(C)C	diisopropyloxalate	1	[15]
COC(=O)CC(=O)OC	dimethylmalonate	3	NIST (Weast)
COC(=O)CC(=O)OC	dimethylmalonate	1	[15]
CCOC(=O)CC(=O)OCC	diethylmalonate	3	NIST (Weast)
CCOC(=O)CC(=O)OCC	diethylmalonate	1	[15]
CCOC(=O)CCC(=O)OCC	diethylsuccinate	1	[15]
CCOC(=O)CCCCC(=O)OCC	diethyladipate	1	[15]

SMILES	name	data type	reference
COC(=O)C=CC(=O)OC	cis-dimethylmaleate	1	[15]
CCOC(=O)C=CC(=O)OCC	cis-diethylmaleate	1	[15]
COC(=O)C=CC(=O)OC	trans-dimethylfumarate	1	[15]
CCOC(=O)C=CC(=O)OCC	trans-diethylfumarate	3	[15]
CCOC(=O)C=CC(=O)OCC	trans-diethylfumarate	1	[15]
carbonyl esters			
CC(=O)CC(=O)OCC	ethyl-3-oxobutanoate	1	[15]
CC(=O)CCC(=O)OC	methyl-4-oxopentanoate	1	[15]
CC(=O)CCC(=O)OCC	ethyl-4-oxopentanoate	3	[15]
CC(=O)CCC(=O)OCC	ethyl-4-oxopentanoate	1	[15]
CC(=O)C(=O)OC	methyl-2-oxopropanoate	3	NIST (Weast)
CC(=O)CC(=O)OC	methyl-3-oxobutanoate	3	NIST (avg)
CC(=O)C(=O)OCC	ethyl-2-oxopropanoate	3	NIST (Lecat)
CCC(=O)C(=O)OCC	ethyl-2-oxobutanoate	3	NIST (Weast)
CC(=O)CC(=O)OCCC	propyl-3-oxobutanoate	3	NIST (ATK)
CC(=O)C(C)C(=O)OCC	ethyl-2-methyl-3-oxobutanoate	3	NIST (Weast)
CC(=O)CCCC(=O)OCC	ethyl-5-oxohexanoate	3	NIST (Aldrich)
CC(=O)CC(=O)OC(C)CC	sec-butyl-3-oxobutanoate	3	NIST (ATK)
CC(=O)CCC(=O)OCCCC	butyl-4-oxopentanoate	3	NIST (Weast)
carbonyl acids			
OC(=O)C(=O)C	2-oxopropanoicacid	1	[15]
OC(=O)C(=O)CC	2-oxobutanoicacid	4	NIST (Aldrich)
OC(=O)C(=O)CC	2-oxobutanoicacid	4	[16]
OC(=O)C(=O)CCC	2-oxopentanoicacid	4	[35]
OC(=O)C(=O)CCC	2-oxopentanoicacid	3	[16]
OC(=O)CCC(=O)C	4-oxopentanoicacid	1	[15]
OC(=O)C(=O)C(C)C	3-methyl-2-oxobutanoicacid	3	EPI

SMILES	name	data type	reference
OC(=O)CCCC(=O)C	5-oxohexanoicacid	3	NIST (Weast)
OC(=O)C(=O)C(C)CC	3-methyl-2-oxopentanoicacid	3	[38]
OC(=O)C(=O)CC(C)C	4-methyl-2-oxopentanoicacid	4	[16]
OC(=O)C(=O)CC(C)C	4-methyl-2-oxopentanoicacid	4	[35]
OC(=O)C(C)CC(=O)C	2-methyl-4-oxopentanoicacid	4	[16]
OC(=O)CC(C)C(=O)C	3-methyl-4-oxopentanoicacid	3	[16]
OC(=O)C(=O)C(C)(C)C	3,3-dimethyl-2-oxobutanoicacid	4	NIST (Weast)
OC(=O)C(=O)C(C)(C)C	3,3-dimethyl-2-oxobutanoicacid	3	[16]
OC(=O)CCCCC(=O)C	6-oxoheptanoicacid	4	NIST (Weast)
OC(=O)CCCCC(=O)C	6-oxoheptanoicacid	4	[35]
OC(=O)C(C)(C)CC(=O)C	2,2-dimethyl-4-oxopentanoicacid	4	[16]
OC(=O)C(=O)CCCCCC	2-oxooctanoicacid	4	[35]
OC(=O)CCCCCC(=O)C	7-oxooctanoicacid	4	[35]
OC(=O)C(C)(C)CCCC(=O)C	2,2-dimethyl-6-oxoheptanoicacid	4	[16]
OC(=O)C(C)(C)CCCC(=O)C	2,2-dimethyl-6-oxoheptanoicacid	3	[16]
OC(=O)CCC(C)(C)CC(=O)C	4,4-dimethyl-6-oxoheptanoicacid	4	[16]
OC(=O)CCC(C)C(=O)C	4-methyl-5-oxohexanoicacid	4	[16]
hydroxy ethers			
OCCOC	2-methoxyethanol	1	[15]
OCCOCC	2-ethoxyethanol	1	[15]
OCCOCCC	2-propoxyethanol	1	[15]
OCCOC(C)C	2-isopropoxyethanol	1	[15]
OCCOCCCC	2-butoxyethanol	1	[15]
OCCOCC(C)C	2-isobutoxyethanol	1	[15]
COCC(O)C	1-methoxy-2-propanol	3	NIST (Aldrich)
COCC(O)C	1-methoxy-2-propanol	1	[64]
OCCCOC	3-methoxy-1-propanol	3	NIST (Smith)

SMILES	name	data type	reference
OCCCOCC	3-ethoxy-1-propanol	3	NIST (Smith)
OCCC(C)OC	3-methoxy-1-butanol	3	NIST (Doering)
OCCCC(C)OC	4-methoxy-1-pentanol	3	NIST (Doering)
hydroxy nitrates			
O=N(=O)OCCO	2-nitrooxyethanol	4	[7]
O=N(=O)OCCO	2-nitrooxyethanol	4	[65]
O=N(=O)OCC(C)O	nitrooxypropanol	4	[65]
O=N(=O)OCCCO	3-nitrooxypropanol	4	[6]
O=N(=O)OC(C)C(C)O	3-nitrooxy-2-butanol	4	[65]
hydroxy peroxides			
CC(C)(C)OOCCO	t-butyl-2-hydroxyethylperoxide	4	[22]
hydroxy carbonyls			
OCC(=O)C	1-hydroxy-2-propanone	3	NIST (Weast)
OCC(=O)C	1-hydroxy-2-propanone	4	[12]
O=CCC(O)C	3-hydroxybutanal	4	[16]
OCC(=O)CC	1-hydroxy-2-butanone	3	NIST (Weast)
CC(=O)C(O)C	3-hydroxy-2-butanone	3	NIST (Weast)
CC(=O)C(O)C	3-hydroxy-2-butanone	4	NIST (Weast)
CC(=O)C(O)C	3-hydroxy-2-butanone	1	[66]
CC(=O)C(O)C	3-hydroxy-2-butanone	2	[67]
CC(=O)CCO	4-hydroxy-2-butanone	4	NIST (Weast)
O=CC(C)(C)CO	2,2-dimethyl-3-hydroxypropanal	4	NIST (Aldrich)
OCC(=O)CCC	1-hydroxy-2-pentanone	3	[16]
CC(=O)C(O)CC	3-hydroxy-2-pentanone	3	[16]
CC(=O)CC(O)C	4-hydroxy-2-pentanone	3	NIST (Sabatier)
CC(=O)CC(O)C	4-hydroxy-2-pentanone	1	[33]
CC(=O)CCCO	5-hydroxy-2-pentanone	3	EPI

SMILES	name	data type	reference
CC(=O)CCCO	5-hydroxy-2-pentanone	4	NIST (Weast)
CC(=O)CCCO	5-hydroxy-2-pentanone	4	[16]
CC(O)C(=O)CC	2-hydroxy-3-pentanone	3	[16]
CC(=O)C(O)(C)C	3-hydroxy-3-methyl-2-butanone	3	NIST (Weast)
CC(=O)C(O)(C)C	3-hydroxy-3-methyl-2-butanone	1	NIST (Conner)
CC(=O)C(C)CO	4-hydroxy-3-methyl-2-butanone	1	NIST (Stull)
CC(=O)C(C)CO	4-hydroxy-3-methyl-2-butanone	4	NIST (Weast)
CC(=O)CC(O)(C)C	4-hydroxy-4-methyl-2-pentanone	3	NIST (Weast)
CC(=O)CC(O)(C)C	4-hydroxy-4-methyl-2-pentanone	1	[2]
CC(=O)CC(O)(C)C	4-hydroxy-4-methyl-2-pentanone	1	[66]
CC(O)(C)C(=O)CCC	2-hydroxy-2-methyl-3-hexanone	3	[33]
CC(O)(C)C(=O)CCC	2-hydroxy-2-methyl-3-hexanone	1	[33]
CCCC(=O)C(O)CCC	5-hydroxy-4-octanone	3	NIST (Weast)
O=C1C(O)(C)C(C2)C(C)(C)C2C1	(1S,2S,5S)-2-hydroxy-3-pinanone	3	[35]
O=C1C(O)(C)C(C2)C(C)(C)C2C1	(1S,2S,5S)-2-hydroxy-3-pinanone	4	[19]
hydroxy acids			
OC(=O)CO	hydroxyaceticacid	6	[68]
OC(=O)C(O)C	2-hydroxypropanoicacid	1	[69]
OC(=O)C(O)C	2-hydroxypropanoicacid	4	NIST (Aldrich)
OC(=O)C(O)CC	2-hydroxybutanoicacid	4	[16]
OC(=O)CC(O)C	3-hydroxybutanoicacid	4	[16]
OC(=O)C(C)(O)C	2-hydroxy-2-methylpropanoicacid	1	[15]
OC(=O)C(O)C(C)C	2-hydroxy-3-methylbutanoicacid	4	[35]
OC(=O)CC(O)(C)C	3-hydroxy-3-methylbutanoicacid	4	[35]
OC(=O)CCCCCO	6-hydroxyhexanoicacid	1	[2]
OC(=O)C(O)CCCCCC	2-hydroxyoctanoicacid	4	[16]
OC1(C(C(=O)O)CC)CCCCC1	cyclobutyrol	4	[16]

SMILES	name	data type	reference
> 2 *functionalities* polyols			
OCC(O)CO	1,2,3-propanetriol	3	NIST (Lecat)
OCC(O)CO	1,2,3-propanetriol	1	[70]
OCC(O)C(O)C	1,2,3-butanetriol	1	NIST (Stull)
OCC(CO)(CO)CC	2-ethyl-2-hydroxymethyl-1,3-propanediol	3	ICSC
OCC(CO)(CO)CC	2-ethyl-2-hydroxymethyl-1,3-propanediol	1	[2]
OCC(O)C(O)CO	erythritol	6	[71, 71, 71]
OCC(O)C(O)CO	erythritol	1	[71]
OCC(O)C(O)CO	erythritol	1	[72]
OCC(O)C(O)CO	erythritol	1	[73]
OCC(O)C(O)CO	threitol	1	[73]
OCC(CO)(CO)CO	pentaerythritol	6	[72, 72, 72]
OCC(CO)(CO)CO	pentaerythritol	6	[74, 72, 72]
OCC(CO)(CO)CO	pentaerythritol	6	[75, 72, 72]
OCC(O)C(O)C(O)CO	adonitol	1	[72]
OCC(O)C(O)C(O)CO	D-arabinitol	1	[72]
OCC(O)C(O)C(O)CO	xylitol	1	[72]
OCC(O)C(O)C(O)C(O)CO	sorbitol	1	[72]
OCC(O)C(O)C(O)C(O)CO	galacticol	1	[72]
OCC(O)C(O)C(O)C(O)CO	D-mannitol	1	[72]
OC1C(O)C(O)C(O)C(O)C1O	myo-inositol	6	[72, 72, 72]
OC1C(O)C(O)C(O)C(O)C1O	myo-inositol	1	[72]
OC1C(O)C(O)C(O)C(O)C1O	myo-inositol	6	[76, 72, 72]
polynitrates			
O=N(=O)OCC(ON(=O)=O)CON(=O)=O	glyceroltrinitrate	2	[39]
O=N(=O)OCC(ON(=O)=O)CON(=O)=O	glyceroltrinitrate	2	[40]
O=N(=O)OCC(ON(=O)=O)CCON(=O)=O	1,2,4-trinitroxybutane	2	[40]

SMILES	name	data type	reference
O=N(=O)OCC(ON(=O)=O)CCCON(=O)=O	1,2,5-trinitroxypentane	2	[40]
O=N(=O)OCC(C)(CON(=O)=O)CON(=O)=O	metrioltrinitrate	1	[77]
O=N(=O)OCC(CON(=O)=O)(CON(=O)=O)CON(=O)=O	pentaerythritoltetranitrate	1	[2]
O=N(=O)OCC(CON(=O)=O)(CON(=O)=O)CON(=O)=O	pentaerythritoltetranitrate	6	[78, 79, 79]
at least 2 acids			
OC(=O)C(O)C(=O)O	2-hydroxypropanoicdiacid	6	[53, 53, 53]
OC(=O)C(O)CC(=O)O	2-hydroxybutanoicdiacid	1	[2]
OC(=O)C(O)CC(=O)O	2-hydroxybutanoicdiacid	6	[53, 53, 53]
OC(=O)C(O)(C)CC(=O)O	2-methyl-2-hydroxybutanoicdiacid	6	[53, 53, 53]
OC(=O)C(O)C(O)C(=O)O	2,3-dihydroxybutanoicdiacid	1	[2]
OC(=O)C(O)C(O)C(=O)O	2,3-dihydroxybutanoicdiacid	6	[53, 53, 53]
OC(=O)CC(O)(C(=O)O)CC(=O)O	3-carboxylic-3-hydroxypentanoicdiacid	1	[2]
OC(=O)CC(O)(C(=O)O)CC(=O)O	3-carboxylic-3-hydroxypentanoicdiacid	6	[53, 53, 53]
OC(=O)C(=O)CC(=O)O	2-oxobutanoicdiacid	6	[53, 53, 53]
OC(=O)C(=O)CCC(=O)O	2-oxopentanoicdiacid	6	[53, 53, 53]
OC(=O)C(=O)CCC(=O)O	2-oxopentanoicdiacid	6	[80, 53, 53]
OC(=O)C(=O)CCC(=O)O	2-oxopentanoicdiacid	7	[81, 53, 53]
OC(=O)CC(=O)CC(=O)O	3-oxopentanoicdiacid	6	[53, 53, 53]
OC(=O)CC(=O)CC(=O)O	3-oxopentanoicdiacid	6	
OC(=O)C(=O)CCCC(=O)O	2-oxohexanoicdiacid	6	[80, 51, 51]
OC(=O)CC(=O)CCC(=O)O	3-oxohexanoicdiacid	6	[80, 51, 51]
OC(=O)CCC(=O)CCC(=O)O	4-oxoheptanoicdiacid	7	[81, 81, 51]
OC(=O)CCCC(=O)CCCC(=O)O	5-oxononanoicdiacid	6	[80, 51, 51]
other polyfunctionals			
O=N(=O)OCCOCCON(=O)=O	diethyleneglycoldinitrate	2	[39]

SMILES	name	data type	reference
O=N(=O)OCCOCCOCCON(=O)=O	triethyleneglycoldinitrate	1	[77]
OC(=O)C(=O)CC(=O)C	2,4-dioxopentanoicacid	4	[16]
OC(=O)C(=O)CO	3-hydroxy-2-oxopropanoicacid	3	[38]
OC1C2COC(O2)C(O)C1O	levoglucosan	7	[62, 62, 62]

2 Remarks on the data

NIST: data taken from the NIST site [82]. NIST (Scott) means that the first author of the data is Scott. NIST (avg) means that an average value over several references was taken.

The data kind is explained in Table 2.

Table 2: Explanation data type numbers.

data type number	data type
1	Liquid vapor pressure correlation.
2	Liquid vapor pressure data set.
3	Boiling point at atmospheric pressure.
4	Boiling point at reduced pressure.
5	Liquid vapor pressure correlation, corrected for gas-phase association.[a]
6	Sublimation pressure correlation, converted to subcooled liquid using fusion properties.[b]
7	Sublimation pressure data set, converted to subcooled liquid using fusion properties.[b]
8	Reported as sublimation pressure correlation, but we assume that it actually refers to the liquid state.
9	Liquid vapor pressure derived from Henry's law constant (see main article).

a. See the second reference for the gas-phase association constant.
b. See the second reference for the fusion temperature, and the third for the fusion enthalpy. Citing ref. [51] means that no experimantal value was available, and that the property was estimated by the method described in this work.

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3 Application examples of EVAPORATION

Only the full model is considered here. For some examples the descriptor assignment is explained.

3.1 Hydrocarbons

Hydrocarbons can be described by the first three descriptors only.

Table 3: Descriptor assignment and estimated $\log_{10}\left(\frac{p^0}{\text{atm}}\right)$ with EVAPORATION (full method) for some example hydrocarbons. $c_1 = 1$ always holds and hence is not given.

SMILES	name	descriptor	$\log_{10}\left(\frac{p^0_{\text{est.}}}{\text{atm}}\right)$ at 298.15 K
CCCC	butane	$c_2 = 4$	0.299
CC(C)C	2-methylpropane	$c_2 = 4, c_3 = 1$	0.499
CC(C)(C)CC[1]	2,2-dimethylbutane	$c_2 = 6, c_3 = 2$	-0.272
CC(C)C(C)C[1]	2,3-dimethylbutane	$c_2 = 6, c_3 = 2$	-0.272
CC(C)(C)C(C)(C)C	2,2,3,3-tetramethylbutane	$c_2 = 8, c_3 = 4$	-0.844
C1CCCCC1[2]	cyclohexane	$c_2 = 6, c_3 = -1$	-0.870
CC1CCCC1 [3]	methylcyclopentane	$c_2 = 6, c_3 = 0$	-0.671
C1CCCC(C1)C2CCCCC2[3]	bicyclohexyl	$c_2 = 12, c_3 = 0$	-3.581
C=CC(C)(C)C	3,3-dimethyl-1-butene	$c_2 = 6, c_3 = 2$	-0.272
CC(C)=C(C)C[4]	2,3-dimethyl-2-butene	$c_2 = 6, c_3 = 0$	0.671
CC1(C)C2C(C)=CCC1C2	α-pinene	$c_2 = 10, c_3 = 2$	-2.213

1. 2,2-dimethylbutane and 2,3-dimethylbutane have both 6 carbon atoms ($c_2 = 6$), and two branchings ($t = c_3 = 2$), hence EVAPORATION will predict the same vapour pressure for them.

2. Cyclohexane has 6 carbon atoms ($c_2 = 6$) and one ring ($c_3 = t = -1$).

3. Methylcyclopentane has 6 carbon atoms($c_2 = 6$), one branching and one ring ($c_3 = t = 1 - 1 = 0$). Bicyclohexyl has two branchings and two rings, so also here $c_3 = 0$.

4. Branchings at double bonds do not count, hence $c_3 = 0$.

3.2 Monofunctional compounds

Note again that only the full model (Sec. 4.3 and Table 4) is considered here, not the model applicable to hydrocarbons and monofunctional compounds (Section 4.2.2 and Table 2).

Table 4: Descriptor assignment and estimated $\log_{10}\left(\frac{p^0}{\text{atm}}\right)$ with EVAPORATION (full method) for some example monofunctional compounds. $c_1 = 1$ always holds and hence is not given.

SMILES	descriptor	$\log_{10}\left(\frac{p^0_{\text{est}}}{\text{atm}}\right)$ at 298.15 K
O=CCCCCC[1]	$c_2 = 6, c_5 = 1, N_{\text{CL}} = 1$	-1.865
CCC(=O)CCC[1]	$c_2 = 6, c_5 = 1, N_{\text{CL}} = 1$	-1.865
CC(=O)C=C[2]	$c_2 = 4, c_5 = 1, c_{13} = 1, N_{\text{CL}} = 1$	-1.078
O=C1CCCCC1[3]	$c_2 = 6, c_3 = -1, c_5 = 1,$ $c_{12} = 1, N_{\text{CL}} = 1$	-2.364
O=C1C=C(C)CC(C)(C)C1	$c_2 = 9, c_3 = 1, c_5 = 1,$ $c_{12} = 1, c_{13} = 1, N_{\text{CL}} = 1$	-3.604
COCCCCC[4]	$c_2 = 7$	-1.156
CCOCCCC[4]	$c_2 = 7$	-1.156
CCC(=O)OCCCC[5]	$c_2 = 8, c_6 = 1, N_{\text{CL}} = 1$	-2.330
C=C(C)C(=O)OC	$c_2 = 6, c_6 = 1, N_{\text{CL}} = 1$	-1.360
C1COOCC1[6]	$c_2 = 6, c_3 = -1, c_{12} = 1$	-1.170
O=N(=O)OC(C)(C)CC	$c_2 = 5, c_3 = 2, c_4 = 1$	-2.153
O=N(=O)OOC(=O)C(C)C	$c_2 = 4, c_3 = 1, c_7 = 1, N_{\text{CL}} = 1$	-2.127
OCC(C)=CC[7]	$c_2 = 5, c_8 = 1, c_{15} = 1, N_{\text{HB}} = 1$	-2.241
CC(O)CCCC[8]	$c_2 = 6, c_8 = 1, c_{14} = 1, N_{\text{HB}} = 1$	-2.423
CC(O)(C)CC(C)(C)C[9]	$c_2 = 8, c_3 = 3, c_8 = 1,$ $c_{14} = 2, N_{\text{HB}} = 1$	-2.260
OC1C(C)CC(C)C1	$c_2 = 7, c_3 = 1, c_8 = 1,$ $c_{12} = 1, c_{14} = 1, N_{\text{HB}} = 1$	-3.010
OC(=O)CCCC	$c_2 = 5, c_9 = 1, N_{\text{HB}} = 1$	-3.798
OC(=O)C1CCCCC1	$c_2 = 7, c_9 = 1, N_{\text{HB}} = 1$	-4.768
OC(=O)CC1CCCC1	$c_2 = 7, c_9 = 1, N_{\text{HB}} = 1$	-4.768
OOC(C)(C)C	$c_2 = 4, c_3 = 2, c_{10} = 1, N_{\text{HB}} = 1$	-2.128
OOC(=O)CCC	$c_2 = 4, c_{11} = 1, N_{\text{HB}} = 1$	-2.396

1. Aldehydic and ketone functionalities are considered as the same group, hence $c_5 = 1$.
2. The ketone functionality is conjugated with a double bond, so $c_{13} = 1$.
3. The functionality is placed on a ring, so $c_{12} = 1$.
4. Ethers have no separate group assignment, but are counted together with the carbon atoms.
5. The in-chain oxygen atom of the ester group is counted together with the carbon atoms.

6. The peroxide group has no separate group assignment; both in-chain oxygen atoms are counted together with the carbon atoms. But its placement within a ring results in $c_{12} = 1$.

7. The alcohol is alkenoic, hence $c_{15} = 1$. This number is never higher than 1.

8. A secondary alcohol, hence $c_{14} = 1$.

9. A tertiary alcohol, hence $c_{14} = 2$.

3.3 Polyfunctional compounds

Apart from descriptor assignment explanation, also some examples are given how to calculate A and B, as for polyfunctional molecules non-additive effects come into play.

Table 5: Descriptor assignment and estimated $\log_{10}\left(\frac{p^0}{\text{atm}}\right)$ with EVAPORATION (full method) for some example polyfunctional compounds. $c_1 = 1$ always holds and hence is not given.

SMILES	descriptor	$\log_{10}\left(\frac{p^0_{\text{est}}}{\text{atm}}\right)$ at 298.15 K
CC(=O)CC(=O)CC[1]	$c_2 = 6, c_5 = 2, c_{17} = 2, N_{\text{CL}} = 2$	-2.644
O=CC(=O)C[2]	$c_2 = 3, c_5 = 2, c_{16} = 2, N_{\text{CL}} = 2$	-0.717
OCCO	$c_2 = 2, c_8 = 2, c_{19} = 2, N_{\text{HB}} = 2$	-3.615
OCC(C)CO	$c_2 = 4, c_3 = 1, c_8 = 2, N_{\text{HB}} = 2$	-4.638
OCC=CCO	$c_2 = 4, c_8 = 2, c_{15} = 1, N_{\text{HB}} = 2$	-4.504
OCC(O)CCC	$c_2 = 5, c_8 = 2, c_{14} = 1, c_{19} = 2, N_{\text{HB}} = 2$	-4.452
OCC(O)CO	$c_2 = 3, c_8 = 3, c_{14} = 1, c_{19} = 4, N_{\text{HB}} = 3$	-6.112
OCC(O)C(O)C(O)CO[3]	$c_2 = 5, c_8 = 5, c_{14} = 3, c_{19} = 8, N_{\text{HB}} = 5$	-11.101
OC(=O)C(=O)O	$c_2 = 2, c_9 = 2, N_{\text{HB}} = 2$	-6.532
OC(=O)C(C)C(=O)O	$c_2 = 4, c_3 = 1, c_9 = 2, N_{\text{HB}} = 2$	-7.303
O=N(=O)OCCON(=O)=O	$c_2 = 2, c_4 = 2$	-3.462
CC(=O)C(O)CC[4]	$c_2 = 5, c_5 = 1, c_8 = 1, c_{14} = 1,$ $c_{18} = 1, c_{19} = 1, N_{\text{CL}} = 1, N_{\text{HB}} = 1$	-2.590
CC(=O)CC(O)C	$c_2 = 5, c_5 = 1, c_8 = 1, c_{14} = 1, N_{\text{CL}} = 1, N_{\text{HB}} = 1$	-3.132
OC(=O)C(=O)C	$c_2 = 3, c_5 = 1, c_9 = 1, c_{20} = 1, N_{\text{CL}} = 1, N_{\text{HB}} = 1$	-3.209
OC(=O)CCCCC(=O)C	$c_2 = 7, c_5 = 1, c_9 = 1, N_{\text{CL}} = 1, N_{\text{HB}} = 1$	-5.962
OC(=O)C(O)C	$c_2 = 3, c_8 = 1, c_9 = 1, c_{14} = 1, c_{19} = 1, N_{\text{HB}} = 2$	-4.941
CCOCOCC	$c_2 = 7$	-1.156
OCCOC	$c_2 = 4, c_8 = 1, c_{19} = 1, N_{\text{HB}} = 1$	-1.875
CCCOC(=O)C(=O)OCCC	$c_2 = 10, c_6 = 2, N_{\text{CL}} = 2$	-4.178
CC(=O)C(=O)OCC[5]	$c_2 = 6, c_5 = 1, c_6 = 1, c_{16} = 1, N_{\text{CL}} = 2$	-2.205
CC(=O)CC(=O)OCCC	$c_2 = 8, c_5 = 1, c_6 = 1, c_{17} = 1, N_{\text{CL}} = 2$	-3.411
O=N(=O)OCCO	$c_2 = 2, c_4 = 1, c_8 = 1, c_{19} = 1, N_{\text{HB}} = 1$	-3.271
O=N(=O)OCCCO	$c_2 = 3, c_4 = 1, c_8 = 1, N_{\text{HB}} = 1$	-3.870
OC(=O)C(=O)CO[6]	$c_2 = 3, c_5 = 1, c_8 = 1, c_9 = 1, c_{18} = 1,$ $c_{19} = 1, c_{20} = 1, N_{\text{CL}} = 1, N_{\text{HB}} = 2$	-5.646
OC(=O)C(O)C(O)C(=O)O[7]	$c_2 = 4, c_8 = 2, c_9 = 2, c_{14} = 2, c_{19} = 4, N_{\text{HB}} = 4$	-7.404
OC(=O)C(=O)CC(=O)O	$c_2 = 4, c_5 = 1, c_9 = 2, c_{20} = 1, N_{\text{CL}} = 1, N_{\text{HB}} = 2$	-6.909
OC(=O)CC(=O)CC(=O)O	$c_2 = 5, c_5 = 1, c_9 = 2, N_{\text{CL}} = 1, N_{\text{HB}} = 2$	-7.982

1. For both carbonyls it holds that a carbonyl-like group is present at the β-position, hence $c_{17} = 2$.

2. For both carbonyls it holds that a carbonyl-like group is present at the α-position, hence $c_{16} = 2$. Calculation: $A = a_1 + 3a_2 + \frac{2a_5 + 2a_{16}}{2^{0.5}} = 3.473, B = b_1 + 3b_2 + 2b_5 + 2b_{16} = -21573$. $A + B/298.15^{1.5} = -0.717$

3. For two hydroxyls, there is one functional group at an α-position present. For three other hydroxyls, there are two functional group at an α-position

present. Hence in total $c_{19} = 8$. Calculation: $A = a_1 + 5a_2 + \frac{5a_8+3a_{14}+8a_{19}}{5^{0.5}} = 4.553, B = -80588$.

4. For the carbonyl there is a non-carbonyl-like, nonacid group present at the α-position ($c_{18} = 1$), while for the alcohol there is a functional group present at the α-position ($c_{19} = 1$).

5. For the ketone there is one carbonyl-like group (an ester) at the α-position present. For the ester this group is not considered, so $c_{16} = 1$. Calculation: $A = a_1 + 6a_2 + \frac{a_5+a_6+a_{16}}{2^{0.5}} = 3.561, B = -29685$.

6. For the ketone there is one non-carbonyl-like, nonacid group present at the α-position ($c_{18} = 1$), for the alcohol there is a functional group present at the α-position ($c_{19} = 1$), and for the acid there is one carbonyl-like group present at the α-position ($c_{20} = 1$). Calculation: $A = a_1 + 3a_2 + \frac{a_5+a_{18}}{1^{0.5}} + \frac{a_8+a_9+a_{19}+a_{20}}{2^{0.5}} = 4.377, B = b_1 + 3b_2 + b_5 + b_{18} + b_8 + b_9 + b_{19} + b_{20} = -51598$.

7. As this molecule has more than two functionalities, of which at least two acid functionalities, the correction factor discussed in Sect. 4.3.2 comes into play. $A = a_1 + 4a_2 + \frac{2a_8+2a_9+2a_{14}+4a_{19}}{4^{0.5}} \frac{2.6}{4} = 3.903, B = b_1 + 4b_2 + (2b_8 + 2b_9 + 2b_{14} + 4b_{19}) \frac{2.6}{4} = -58212$.