Supplementary material

April 21, 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=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] |
| 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=CCC | 2-methylpentenoicacid | 3 | [16] |
| OC(=O)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)C(C)C=CC | 2-methyl-3-pentenoicacid | 3 | [16] |
| 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) |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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] |
| 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 | [38] |
| O=N(=O)OCC(C)ON(=O)=O | 1,2-propylenedinitrate | 2 | [38] |
| O=N(=O)OCCCON(=O)=O | 1,3propylenedinitrate | 2 | [38] |
| O=N(=O)OCCCON(=O)=O | 1,3propylenedinitrate | 2 | [39] |
| O=N(=O)OCCCCON(=O)=O | 1,4-dinitroxybutane | 2 | [39] |
| O=N(=O)OCCC(C)ON(=O)=O | 1,3-dinitroxybutane | 2 | [39] |
| O=N(=O)OCCCCCON(=O)=O | 1,5-dinitroxypentane | 2 | [39] |
| O=N(=O)OC(C)CC(C)ON(=O)=O | 2,4-dinitroxypentane | 2 | [39] |
| O=N(=O)OC(C)CCCC(C)ON(=O)=O | 2,5-dinitroxyhexane | 2 | [39] |
| 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] |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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) |
| 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 | [40] |
| 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 | [40] |
| 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] |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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] |
| 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] |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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] |
| 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 | [49] |
| OC(=O)CCC(=O)O | butanoicdiacid | 1 | [54] |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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] |
| 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] |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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] |
| 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] |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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] |
| 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) |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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] |
| 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) |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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 |
| OC(=O)CCCC(=O)C | 5-oxohexanoicacid | 3 | NIST (Weast) |
| OC(=O)C(=O)C(C)CC | 3-methyl-2-oxopentanoicacid | 3 | [40] |
| 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(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) |

| SMILES | name | data type | reference |
|---|---|---|---|
| COCC(O)C | 1-methoxy-2-propanol | 1 | [64] |
| OCCCOC | 3-methoxy-1-propanol | 3 | NIST (Smith) |
| 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) |

| SMILES | name | data type | reference |
|---|---|---|---|
| CC(=O)CC(O)C | 4-hydroxy-2-pentanone | 1 | [33] |
| CC(=O)CCCO | 5-hydroxy-2-pentanone | 3 | EPI |
| 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)C(O)C | 2-hydroxypropanoicacid | 1 | [68] |
| 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)CCCCCO | 6-hydroxyhexanoicacid | 1 | [2] |
| $> 2$ *functionalities* polyols | | | |
| OCC(O)CO | 1,2,3-propanetriol | 3 | NIST (Lecat) |
| OCC(O)CO | 1,2,3-propanetriol | 1 | [69] |

| SMILES | name | data type | reference |
|---|---|---|---|
| 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 | [70, 70, 70] |
| OCC(O)C(O)CO | erythritol | 1 | [70] |
| OCC(O)C(O)CO | erythritol | 1 | [71] |
| OCC(O)C(O)CO | erythritol | 1 | [72] |
| OCC(O)C(O)CO | threitol | 1 | [72] |
| OCC(CO)(CO)CO | pentaerythritol | 6 | [71, 71, 71] |
| OCC(CO)(CO)CO | pentaerythritol | 6 | [73, 71, 71] |
| OCC(CO)(CO)CO | pentaerythritol | 6 | [74, 71, 71] |
| OCC(O)C(O)C(O)CO | adonitol | 1 | [71] |
| OCC(O)C(O)C(O)CO | D-arabinitol | 1 | [71] |
| OCC(O)C(O)C(O)CO | xylitol | 1 | [71] |
| OCC(O)C(O)C(O)C(O)CO | sorbitol | 1 | [71] |
| OCC(O)C(O)C(O)C(O)CO | galacticol | 1 | [71] |
| OCC(O)C(O)C(O)C(O)CO | D-mannitol | 1 | [71] |
| OC1C(O)C(O)C(O)C(O)C1O | myo-inositol | 6 | [71, 71, 71] |
| OC1C(O)C(O)C(O)C(O)C1O | myo-inositol | 1 | [71] |
| OC1C(O)C(O)C(O)C(O)C1O | myo-inositol | 6 | [75, 71, 71] |
| polynitrates | | | |
| O=N(=O)OCC(ON(=O)=O)CON(=O)=O | glyceroltrinitrate | 2 | [38] |
| O=N(=O)OCC(ON(=O)=O)CON(=O)=O | glyceroltrinitrate | 2 | [39] |
| O=N(=O)OCC(ON(=O)=O)CCON(=O)=O | 1,2,4-trinitroxybutane | 2 | [39] |
| O=N(=O)OCC(ON(=O)=O)CCCON(=O)=O | 1,2,5-trinitroxypentane | 2 | [39] |
| O=N(=O)OCC(C)(CON(=O)=O)CON(=O)=O | metrioltrinitrate | 1 | [76] |
| O=N(=O)OCC(CON(=O)=O)(CON(=O)=O)CON(=O)=O | | | |

| SMILES | name | data type | reference |
|---|---|---|---|
| | pentaerythritoltetranitrate | 1 | [2] |
| O=N(=O)OCC(CON(=O)=O)(CON(=O)=O)CON(=O)=O | | | |
| | pentaerythritoltetranitrate | 6 | [77, 78, 78] |
| 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 | 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 | 6 | [53, 53, 53] |
| 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 | [79, 53, 53] |
| OC(=O)C(=O)CCC(=O)O | 2-oxopentanoicdiacid | 7 | [80, 53, 53] |
| OC(=O)CC(=O)CC(=O)O | 3-oxopentanoicdiacid | 6 | [53, 53, 53] |
| OC(=O)C(=O)CCCC(=O)O | 2-oxohexanoicdiacid | 6 | [79, 51, 51] |
| OC(=O)CC(=O)CCC(=O)O | 3-oxohexanoicdiacid | 6 | [79, 51, 51] |
| OC(=O)CCC(=O)CCC(=O)O | 4-oxoheptanoicdiacid | 7 | [80, 80, 51] |
| OC(=O)CCCC(=O)CCCC(=O)O | 5-oxononanoicdiacid | 6 | [79, 51, 51] |
| other polyfunctionals | | | |
| O=N(=O)OCCOCCON(=O)=O | diethyleneglycoldinitrate | 2 | [38] |
| O=N(=O)OCCOCCOCCON(=O)=O | triethyleneglycoldinitrate | 1 | [76] |
| OC(=O)C(=O)CC(=O)C | 2,4-dioxopentanoicacid | 4 | [16] |
| OC(=O)C(=O)CO | 3-hydroxy-2-oxopropanoicacid | 3 | [40] |
| OC1C2COC(O2)C(O)C1O | levoglucosan | 7 | [62, 62, 62] |

## 2 Remarks on the data

NIST: data taken from the NIST site [81]. 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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