# Dimethylmalonic acid, hexadecyl 2,2,3,3-tetrafluoropropyl ester

**Inchi:** InChI=1S/C24H42F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-31-21(29)23(2,3)22

**InchiKey:** ZBQYVJXYLLYKHC-UHFFFAOYSA-N

**Formula:** C24H42F4O4

**SMILES:** CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F

**Mol. weight [g/mol]:** 470.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1092.64 | kJ/mol | Joback Method |
| hf | -1835.51 | kJ/mol | Joback Method |
| hfus | 57.46 | kJ/mol | Joback Method |
| hvap | 81.08 | kJ/mol | Joback Method |
| log10ws | -7.98 | | Crippen Method |
| logp | 7.481 | | Crippen Method |
| mcvol | 370.980 | ml/mol | McGowan Method |
| pc | 787.27 | kPa | Joback Method |
| rinpol | 2403.00 | | NIST Webbook |
| rinpol | 2403.00 | | NIST Webbook |
| tb | 891.28 | K | Joback Method |
| tc | 1094.01 | K | Joback Method |
| tf | 496.76 | K | Joback Method |
| vc | 1.472 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1246.51 | J/mol×K | 891.28 | Joback Method |
| cpg | 1265.88 | J/mol×K | 925.07 | Joback Method |
| cpg | 1283.95 | J/mol×K | 958.86 | Joback Method |
| cpg | 1300.79 | J/mol×K | 992.65 | Joback Method |
| cpg | 1316.49 | J/mol×K | 1026.43 | Joback Method |
| cpg | 1331.10 | J/mol×K | 1060.22 | Joback Method |
| cpg | 1344.71 | J/mol×K | 1094.01 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U361926&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |