# Diethylmalonic acid, 2,2,3,3,3-pentafluoropropyl tetradecyl ester

**Inchi:** InChI=1S/C24H41F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-32-20(30)22(5-2,6-3)21

**InchiKey:** GHMSDZJTPNHTHE-UHFFFAOYSA-N

**Formula:** C24H41F5O4

**SMILES:** CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 488.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1282.17 | kJ/mol | Joback Method |
| hf | -2035.09 | kJ/mol | Joback Method |
| hfus | 56.65 | kJ/mol | Joback Method |
| hvap | 79.36 | kJ/mol | Joback Method |
| log10ws | -8.33 | | Crippen Method |
| logp | 7.778 | | Crippen Method |
| mcvol | 372.750 | ml/mol | McGowan Method |
| pc | 772.46 | kPa | Joback Method |
| rinpol | 2205.00 | | NIST Webbook |
| rinpol | 2205.00 | | NIST Webbook |
| tb | 887.76 | K | Joback Method |
| tc | 1089.87 | K | Joback Method |
| tf | 514.77 | K | Joback Method |
| vc | 1.484 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1253.40 | J/mol×K | 887.76 | Joback Method |
| cpg | 1272.47 | J/mol×K | 921.44 | Joback Method |
| cpg | 1290.30 | J/mol×K | 955.13 | Joback Method |
| cpg | 1307.00 | J/mol×K | 988.81 | Joback Method |
| cpg | 1322.65 | J/mol×K | 1022.50 | Joback Method |
| cpg | 1337.34 | J/mol×K | 1056.18 | Joback Method |
| cpg | 1351.16 | J/mol×K | 1089.87 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370851&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |