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

**Inchi:** InChI=1S/C27H47F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-35-23(33)25(5

**InchiKey:** SWNXFVFJSIVWEF-UHFFFAOYSA-N

**Formula:** C27H47F5O4

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

**Mol. weight [g/mol]:** 530.65

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1256.91 | kJ/mol | Joback Method |
| hf | -2097.01 | kJ/mol | Joback Method |
| hfus | 64.42 | kJ/mol | Joback Method |
| hvap | 86.03 | kJ/mol | Joback Method |
| log10ws | -9.58 | | Crippen Method |
| logp | 8.948 | | Crippen Method |
| mcvol | 415.020 | ml/mol | McGowan Method |
| pc | 662.21 | kPa | Joback Method |
| rinpol | 2499.00 | | NIST Webbook |
| rinpol | 2499.00 | | NIST Webbook |
| tb | 956.40 | K | Joback Method |
| tc | 1186.65 | K | Joback Method |
| tf | 548.58 | K | Joback Method |
| vc | 1.653 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1442.75 | J/mol×K | 956.40 | Joback Method |
| cpg | 1464.27 | J/mol×K | 994.77 | Joback Method |
| cpg | 1484.28 | J/mol×K | 1033.15 | Joback Method |
| cpg | 1502.93 | J/mol×K | 1071.52 | Joback Method |
| cpg | 1520.37 | J/mol×K | 1109.90 | Joback Method |
| cpg | 1536.73 | J/mol×K | 1148.27 | Joback Method |
| cpg | 1552.17 | J/mol×K | 1186.65 | 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=U370854&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 |