# Diethylmalonic acid, heptadecyl pentafluorobenzyl ester

**Inchi:** InChI=1S/C31H47F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-39-29(37)31(5
**InchiKey:** SKZPOKCVJORIBX-UHFFFAOYSA-N
**Formula:** C31H47F5O4
**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 578.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1164.65 | kJ/mol | Joback Method |
| hf | -1982.89 | kJ/mol | Joback Method |
| hfus | 81.70 | kJ/mol | Joback Method |
| hvap | 103.12 | kJ/mol | Joback Method |
| log10ws | -11.54 | | Crippen Method |
| logp | 9.646 | | Crippen Method |
| mcvol | 447.620 | ml/mol | McGowan Method |
| pc | 609.06 | kPa | Joback Method |
| rinpol | 3056.00 | | NIST Webbook |
| tb | 1105.96 | K | Joback Method |
| tc | 1407.69 | K | Joback Method |
| tf | 677.84 | K | Joback Method |
| vc | 1.790 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1589.15 | J/mol×K | 1105.96 | Joback Method |
| cpg | 1609.29 | J/mol×K | 1156.25 | Joback Method |
| cpg | 1626.64 | J/mol×K | 1206.54 | Joback Method |
| cpg | 1641.38 | J/mol×K | 1256.83 | Joback Method |
| cpg | 1653.68 | J/mol×K | 1307.12 | Joback Method |
| cpg | 1663.71 | J/mol×K | 1357.40 | Joback Method |
| cpg | 1671.65 | J/mol×K | 1407.69 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370003&Units=SI |

# 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 |