# Diethylmalonic acid, pentafluorophenyl undecyl ester

**Inchi:** InChI=1S/C24H33F5O4/c1-4-7-8-9-10-11-12-13-14-15-32-22(30)24(5-2,6-3)23(31)33-21
**InchiKey:** DZNJYHKUCLMHAE-UHFFFAOYSA-N
**Formula:** C24H33F5O4
**SMILES:** CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 480.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1223.59 | kJ/mol | Joback Method |
| hf | -1838.41 | kJ/mol | Joback Method |
| hfus | 63.57 | kJ/mol | Joback Method |
| hvap | 87.53 | kJ/mol | Joback Method |
| log10ws | -8.76 | | Crippen Method |
| logp | 7.168 | | Crippen Method |
| mcvol | 348.990 | ml/mol | McGowan Method |
| pc | 875.32 | kPa | Joback Method |
| rinpol | 2380.00 | | NIST Webbook |
| rinpol | 2380.00 | | NIST Webbook |
| tb | 945.80 | K | Joback Method |
| tc | 1160.70 | K | Joback Method |
| tf | 598.95 | K | Joback Method |
| vc | 1.399 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1151.93 | J/mol×K | 945.80 | Joback Method |
| cpg | 1167.96 | J/mol×K | 981.62 | Joback Method |
| cpg | 1182.60 | J/mol×K | 1017.43 | Joback Method |
| cpg | 1195.91 | J/mol×K | 1053.25 | Joback Method |
| cpg | 1207.91 | J/mol×K | 1089.07 | Joback Method |
| cpg | 1218.67 | J/mol×K | 1124.88 | Joback Method |
| cpg | 1228.20 | J/mol×K | 1160.70 | 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=U370218&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 |