# Diethylmalonic acid, 4-fluoro-2-methoxyphenyl undecyl ester

**Inchi:** InChI=1S/C25H39FO5/c1-5-8-9-10-11-12-13-14-15-18-30-23(27)25(6-2,7-3)24(28)31-21
**InchiKey:** VBMMCBUSKLAGPV-UHFFFAOYSA-N
**Formula:** C25H39FO5
**SMILES:** CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)cc1OC
**Mol. weight [g/mol]:** 438.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -512.04 | kJ/mol | Joback Method |
| hf | -1172.42 | kJ/mol | Joback Method |
| hfus | 56.20 | kJ/mol | Joback Method |
| hvap | 93.45 | kJ/mol | Joback Method |
| log10ws | -7.56 | | Crippen Method |
| logp | 6.620 | | Crippen Method |
| mcvol | 361.870 | ml/mol | McGowan Method |
| pc | 936.35 | kPa | Joback Method |
| rinpol | 2758.00 | | NIST Webbook |
| tb | 979.08 | K | Joback Method |
| tc | 1198.89 | K | Joback Method |
| tf | 592.53 | K | Joback Method |
| vc | 1.401 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1217.07 | J/mol×K | 979.08 | Joback Method |
| cpg | 1233.37 | J/mol×K | 1015.72 | Joback Method |
| cpg | 1248.13 | J/mol×K | 1052.35 | Joback Method |
| cpg | 1261.40 | J/mol×K | 1088.99 | Joback Method |
| cpg | 1273.23 | J/mol×K | 1125.62 | Joback Method |
| cpg | 1283.66 | J/mol×K | 1162.26 | Joback Method |
| cpg | 1292.73 | J/mol×K | 1198.89 | 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=U370888&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **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 |

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