# Diethylmalonic acid, 2-chloro-6-fluorophenyl tetradecyl ester

**Inchi:** InChI=1S/C27H42ClFO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-21-32-25(30)27(5-2,6-3)26

**InchiKey:** KLANPTDHODLZSF-UHFFFAOYSA-N

**Formula:** C27H42ClFO4

**SMILES:** CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)cccc1Cl

**Mol. weight [g/mol]:** 485.07

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -402.13 | kJ/mol | Joback Method |
| hf | -1097.22 | kJ/mol | Joback Method |
| hfus | 64.39 | kJ/mol | Joback Method |
| hvap | 99.88 | kJ/mol | Joback Method |
| log10ws | -9.38 | | Crippen Method |
| logp | 8.435 | | Crippen Method |
| mcvol | 396.420 | ml/mol | McGowan Method |
| pc | 825.74 | kPa | Joback Method |
| rinpol | 3095.00 | | NIST Webbook |
| tb | 1039.85 | K | Joback Method |
| tc | 1276.78 | K | Joback Method |
| tf | 622.76 | K | Joback Method |
| vc | 1.544 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1337.95 | J/mol×K | 1039.85 | Joback Method |
| cpg | 1354.55 | J/mol×K | 1079.34 | Joback Method |
| cpg | 1369.60 | J/mol×K | 1118.83 | Joback Method |
| cpg | 1383.18 | J/mol×K | 1158.31 | Joback Method |
| cpg | 1395.38 | J/mol×K | 1197.80 | Joback Method |
| cpg | 1406.30 | J/mol×K | 1237.29 | Joback Method |
| cpg | 1416.02 | J/mol×K | 1276.78 | Joback Method |

# Sources

| | |
|---|---|
| **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=U369684&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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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