# Diethylmalonic acid, 2-fluorophenyl heptadecyl ester

**Inchi:** InChI=1S/C30H49FO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-34-28(32)30(5-

**InchiKey:** IWRDUVBECOFNTL-UHFFFAOYSA-N

**Formula:** C30H49FO4

**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F

**Mol. weight [g/mol]:** 492.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -355.31 | kJ/mol | Joback Method |
| hf | -1131.93 | kJ/mol | Joback Method |
| hfus | 68.35 | kJ/mol | Joback Method |
| hvap | 101.51 | kJ/mol | Joback Method |
| log10ws | -9.95 | | Crippen Method |
| logp | 8.952 | | Crippen Method |
| mcvol | 426.450 | ml/mol | McGowan Method |
| pc | 724.18 | kPa | Joback Method |
| rinpol | 3215.00 | | NIST Webbook |
| tb | 1066.08 | K | Joback Method |
| tc | 1317.90 | K | Joback Method |
| tf | 614.13 | K | Joback Method |
| vc | 1.663 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1503.29 | J/mol×K | 1066.08 | Joback Method |
| cpg | 1522.47 | J/mol×K | 1108.05 | Joback Method |
| cpg | 1539.84 | J/mol×K | 1150.02 | Joback Method |
| cpg | 1555.53 | J/mol×K | 1191.99 | Joback Method |
| cpg | 1569.65 | J/mol×K | 1233.96 | Joback Method |
| cpg | 1582.35 | J/mol×K | 1275.93 | Joback Method |
| cpg | 1593.76 | J/mol×K | 1317.90 | Joback Method |

# Sources

| | |
|---|---|
| **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=U370141&Units=SI |

# 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 |