# Diethylmalonic acid, 2-fluorophenyl propyl ester

**Inchi:** InChI=1S/C16H21FO4/c1-4-11-20-14(18)16(5-2,6-3)15(19)21-13-10-8-7-9-12(13)17/h7-1
**InchiKey:** FDOZITGEMDIAIE-UHFFFAOYSA-N
**Formula:** C16H21FO4
**SMILES:** CCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F
**Mol. weight [g/mol]:** 296.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -473.19 | kJ/mol | Joback Method |
| hf | -842.97 | kJ/mol | Joback Method |
| hfus | 32.09 | kJ/mol | Joback Method |
| hvap | 70.35 | kJ/mol | Joback Method |
| log10ws | -4.09 | | Crippen Method |
| logp | 3.491 | | Crippen Method |
| mcvol | 229.190 | ml/mol | McGowan Method |
| pc | 1777.34 | kPa | Joback Method |
| rinpol | 1810.00 | | NIST Webbook |
| rinpol | 1810.00 | | NIST Webbook |
| tb | 745.76 | K | Joback Method |
| tc | 948.92 | K | Joback Method |
| tf | 456.35 | K | Joback Method |
| vc | 0.878 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 658.33 | J/mol×K | 745.76 | Joback Method |
| cpg | 673.19 | J/mol×K | 779.62 | Joback Method |
| cpg | 687.05 | J/mol×K | 813.48 | Joback Method |
| cpg | 699.93 | J/mol×K | 847.34 | Joback Method |
| cpg | 711.88 | J/mol×K | 881.20 | Joback Method |
| cpg | 722.92 | J/mol×K | 915.06 | Joback Method |
| cpg | 733.07 | J/mol×K | 948.92 | 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=U370126&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 |