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

**Inchi:** InChI=1S/C20H28ClFO4/c1-4-7-8-9-10-14-25-18(23)20(5-2,6-3)19(24)26-17-15(21)12-11

**InchiKey:** NNISHEYQQAHUHW-UHFFFAOYSA-N

**Formula:** C20H28ClFO4

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

**Mol. weight [g/mol]:** 386.88

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -461.07 | kJ/mol | Joback Method |
| hf | -952.74 | kJ/mol | Joback Method |
| hfus | 46.26 | kJ/mol | Joback Method |
| hvap | 84.30 | kJ/mol | Joback Method |
| log10ws | -6.45 | | Crippen Method |
| logp | 5.704 | | Crippen Method |
| mcvol | 297.790 | ml/mol | McGowan Method |
| pc | 1268.25 | kPa | Joback Method |
| rinpol | 2350.00 | | NIST Webbook |
| rinpol | 2350.00 | | NIST Webbook |
| tb | 879.69 | K | Joback Method |
| tc | 1086.28 | K | Joback Method |
| tf | 543.87 | K | Joback Method |
| vc | 1.151 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 912.12 | J/mol×K | 879.69 | Joback Method |
| cpg | 926.72 | J/mol×K | 914.12 | Joback Method |
| cpg | 940.21 | J/mol×K | 948.55 | Joback Method |
| cpg | 952.63 | J/mol×K | 982.99 | Joback Method |
| cpg | 964.02 | J/mol×K | 1017.42 | Joback Method |
| cpg | 974.42 | J/mol×K | 1051.85 | Joback Method |
| cpg | 983.87 | J/mol×K | 1086.28 | 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=U369678&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 |