# Diethylmalonic acid, 3,4-difluorobenzyl hexyl ester

**Inchi:** InChI=1S/C20H28F2O4/c1-4-7-8-9-12-25-18(23)20(5-2,6-3)19(24)26-14-15-10-11-16(21)

**InchiKey:** ZWOQMJBJPJHIJS-UHFFFAOYSA-N

**Formula:** C20H28F2O4

**SMILES:** CCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1

**Mol. weight [g/mol]:** 370.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -643.95 | kJ/mol | Joback Method |
| hf | -1133.11 | kJ/mol | Joback Method |
| hfus | 45.14 | kJ/mol | Joback Method |
| hvap | 79.10 | kJ/mol | Joback Method |
| log10ws | -5.94 | | Crippen Method |
| logp | 4.938 | | Crippen Method |
| mcvol | 287.320 | ml/mol | McGowan Method |
| pc | 1261.06 | kPa | Joback Method |
| rinpol | 2154.00 | | NIST Webbook |
| tb | 841.53 | K | Joback Method |
| tc | 1039.03 | K | Joback Method |
| tf | 514.54 | K | Joback Method |
| vc | 1.121 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 892.81 | J/mol×K | 841.53 | Joback Method |
| cpg | 908.16 | J/mol×K | 874.45 | Joback Method |
| cpg | 922.44 | J/mol×K | 907.36 | Joback Method |
| cpg | 935.68 | J/mol×K | 940.28 | Joback Method |
| cpg | 947.93 | J/mol×K | 973.20 | Joback Method |
| cpg | 959.21 | J/mol×K | 1006.12 | Joback Method |
| cpg | 969.56 | J/mol×K | 1039.03 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369326&Units=SI |
| **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 |

# 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 |