# 2,5-Difluorobenzoic acid, 4-hexadecyl ester

**Inchi:** InChI=1S/C23H36F2O2/c1-3-5-6-7-8-9-10-11-12-13-15-20(14-4-2)27-23(26)21-18-19(24
**InchiKey:** QOCSJXUOMCMANG-UHFFFAOYSA-N
**Formula:** C23H36F2O2
**SMILES:** CCCCCCCCCCCCCC(CCC)OC(=O)c1cc(F)ccc1F
**Mol. weight [g/mol]:** 382.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -390.05 | kJ/mol | Joback Method |
| hf | -946.76 | kJ/mol | Joback Method |
| hfus | 54.01 | kJ/mol | Joback Method |
| hvap | 77.53 | kJ/mol | Joback Method |
| log10ws | -8.77 | | Crippen Method |
| logp | 7.601 | | Crippen Method |
| mcvol | 322.150 | ml/mol | McGowan Method |
| pc | 1000.81 | kPa | Joback Method |
| rinpol | 2413.00 | | NIST Webbook |
| rinpol | 2413.00 | | NIST Webbook |
| tb | 836.67 | K | Joback Method |
| tc | 1027.18 | K | Joback Method |
| tf | 458.77 | K | Joback Method |
| vc | 1.270 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1020.97 | J/mol×K | 836.67 | Joback Method |
| cpg | 1039.23 | J/mol×K | 868.42 | Joback Method |
| cpg | 1056.38 | J/mol×K | 900.17 | Joback Method |
| cpg | 1072.47 | J/mol×K | 931.93 | Joback Method |
| cpg | 1087.52 | J/mol×K | 963.68 | Joback Method |
| cpg | 1101.57 | J/mol×K | 995.43 | Joback Method |
| cpg | 1114.66 | J/mol×K | 1027.18 | Joback Method |

# Sources

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|---|---|
| **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=U338490&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 |