# 2,6-Difluoro-3-methylbenzoic acid, tetradecyl ester

**Inchi:** InChI=1S/C22H34F2O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-26-22(25)20-19(23)16-15-1
**InchiKey:** PZDPWCSZZMISIZ-UHFFFAOYSA-N
**Formula:** C22H34F2O2
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F
**Mol. weight [g/mol]:** 368.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -405.66 | kJ/mol | Joback Method |
| hf | -932.31 | kJ/mol | Joback Method |
| hfus | 54.56 | kJ/mol | Joback Method |
| hvap | 76.35 | kJ/mol | Joback Method |
| log10ws | -8.29 | | Crippen Method |
| logp | 7.131 | | Crippen Method |
| mcvol | 308.060 | ml/mol | McGowan Method |
| pc | 1048.69 | kPa | Joback Method |
| rinpol | 2515.00 | | NIST Webbook |
| rinpol | 2515.00 | | NIST Webbook |
| tb | 819.21 | K | Joback Method |
| tc | 1007.09 | K | Joback Method |
| tf | 475.02 | K | Joback Method |
| vc | 1.220 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 959.62 | J/mol×K | 819.21 | Joback Method |
| cpg | 977.37 | J/mol×K | 850.52 | Joback Method |
| cpg | 994.08 | J/mol×K | 881.84 | Joback Method |
| cpg | 1009.80 | J/mol×K | 913.15 | Joback Method |
| cpg | 1024.53 | J/mol×K | 944.46 | Joback Method |
| cpg | 1038.32 | J/mol×K | 975.78 | Joback Method |
| cpg | 1051.18 | J/mol×K | 1007.09 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U338851&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

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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 |