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

**Inchi:** InChI=1S/C23H36F2O2/c1-4-6-7-8-9-10-11-12-13-14-15-19(5-2)27-23(26)21-20(24)17-1

**InchiKey:** PXRABPPVXNXSJY-UHFFFAOYSA-N

**Formula:** C23H36F2O2

**SMILES:** CCCCCCCCCCCCC(CC)OC(=O)c1c(F)ccc(C)c1F

**Mol. weight [g/mol]:** 382.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -399.68 | kJ/mol | Joback Method |
| hf | -958.23 | kJ/mol | Joback Method |
| hfus | 53.62 | kJ/mol | Joback Method |
| hvap | 78.19 | kJ/mol | Joback Method |
| log10ws | -8.83 | | Crippen Method |
| logp | 7.520 | | Crippen Method |
| mcvol | 322.150 | ml/mol | McGowan Method |
| pc | 991.38 | kPa | Joback Method |
| rinpol | 2515.00 | | NIST Webbook |
| rinpol | 2515.00 | | NIST Webbook |
| tb | 841.65 | K | Joback Method |
| tc | 1033.14 | K | Joback Method |
| tf | 471.29 | K | Joback Method |
| vc | 1.270 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1020.79 | J/mol×K | 841.65 | Joback Method |
| cpg | 1038.98 | J/mol×K | 873.56 | Joback Method |
| cpg | 1056.07 | J/mol×K | 905.48 | Joback Method |
| cpg | 1072.08 | J/mol×K | 937.39 | Joback Method |
| cpg | 1087.04 | J/mol×K | 969.31 | Joback Method |
| cpg | 1100.99 | J/mol×K | 1001.22 | Joback Method |
| cpg | 1113.95 | J/mol×K | 1033.14 | Joback Method |

# Sources

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|---|---|
| **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=U338591&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |