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

**Inchi:** InChI=1S/C28H46F2O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-32-28(3

**InchiKey:** QEFDIZQXWJOHMF-UHFFFAOYSA-N

**Formula:** C28H46F2O2

**SMILES:** CCCCCCCCCCCCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F

**Mol. weight [g/mol]:** 452.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -355.14 | kJ/mol | Joback Method |
| hf | -1056.15 | kJ/mol | Joback Method |
| hfus | 70.10 | kJ/mol | Joback Method |
| hvap | 89.71 | kJ/mol | Joback Method |
| log10ws | -10.81 | | Crippen Method |
| logp | 9.472 | | Crippen Method |
| mcvol | 392.600 | ml/mol | McGowan Method |
| pc | 744.88 | kPa | Joback Method |
| rinpol | 3186.00 | | NIST Webbook |
| tb | 956.49 | K | Joback Method |
| tc | 1175.43 | K | Joback Method |
| tf | 542.64 | K | Joback Method |
| vc | 1.556 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1333.55 | J/mol×K | 956.49 | Joback Method |
| cpg | 1354.11 | J/mol×K | 992.98 | Joback Method |
| cpg | 1373.14 | J/mol×K | 1029.47 | Joback Method |
| cpg | 1390.70 | J/mol×K | 1065.96 | Joback Method |
| cpg | 1406.85 | J/mol×K | 1102.45 | Joback Method |
| cpg | 1421.65 | J/mol×K | 1138.94 | Joback Method |
| cpg | 1435.18 | J/mol×K | 1175.43 | 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=U338857&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 |