# 2,6-Difluoro-3-methylbenzoic acid, 4-benzyloxyphenyl ester

**Inchi:** InChI=1S/C21H16F2O3/c1-14-7-12-18(22)19(20(14)23)21(24)26-17-10-8-16(9-11-17)25-

**InchiKey:** HWOHMPVKLMSDKK-UHFFFAOYSA-N

**Formula:** C21H16F2O3

**SMILES:** Cc1ccc(F)c(C(=O)Oc2ccc(OCc3ccccc3)cc2)c1F

**Mol. weight [g/mol]:** 354.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -303.89 | kJ/mol | Joback Method |
| hf | -582.30 | kJ/mol | Joback Method |
| hfus | 40.85 | kJ/mol | Joback Method |
| hvap | 81.75 | kJ/mol | Joback Method |
| log10ws | -6.93 | | Crippen Method |
| logp | 5.071 | | Crippen Method |
| mcvol | 252.320 | ml/mol | McGowan Method |
| pc | 1792.42 | kPa | Joback Method |
| rinpol | 2810.00 | | NIST Webbook |
| tb | 877.09 | K | Joback Method |
| tc | 1111.02 | K | Joback Method |
| tf | 551.34 | K | Joback Method |
| vc | 0.966 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 738.56 | J/mol×K | 877.09 | Joback Method |
| cpg | 751.59 | J/mol×K | 916.08 | Joback Method |
| cpg | 763.29 | J/mol×K | 955.07 | Joback Method |
| cpg | 773.69 | J/mol×K | 994.05 | Joback Method |
| cpg | 782.83 | J/mol×K | 1033.04 | Joback Method |
| cpg | 790.75 | J/mol×K | 1072.03 | Joback Method |
| cpg | 797.49 | J/mol×K | 1111.02 | 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=U357688&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 |