# 2,6-Difluorobenzoic acid, 3-methylbut-2-enyl ester

**Inchi:** InChI=1S/C12H12F2O2/c1-8(2)6-7-16-12(15)11-9(13)4-3-5-10(11)14/h3-6H,7H2,1-2H3
**InchiKey:** YQNYJIWZPQVFMT-UHFFFAOYSA-N
**Formula:** C12H12F2O2
**SMILES:** CC(C)=CCOC(=O)c1c(F)cccc1F
**Mol. weight [g/mol]:** 226.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -408.56 | kJ/mol | Joback Method |
| hf | -607.01 | kJ/mol | Joback Method |
| hfus | 27.94 | kJ/mol | Joback Method |
| hvap | 53.47 | kJ/mol | Joback Method |
| log10ws | -3.91 | | Crippen Method |
| logp | 3.088 | | Crippen Method |
| mcvol | 162.860 | ml/mol | McGowan Method |
| pc | 2365.67 | kPa | Joback Method |
| rinpol | 1481.30 | | NIST Webbook |
| tb | 589.47 | K | Joback Method |
| tc | 790.29 | K | Joback Method |
| tf | 330.76 | K | Joback Method |
| vc | 0.640 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 389.54 | J/mol×K | 589.47 | Joback Method |
| cpg | 402.53 | J/mol×K | 622.94 | Joback Method |
| cpg | 414.79 | J/mol×K | 656.41 | Joback Method |
| cpg | 426.36 | J/mol×K | 689.88 | Joback Method |
| cpg | 437.26 | J/mol×K | 723.35 | Joback Method |
| cpg | 447.51 | J/mol×K | 756.82 | Joback Method |
| cpg | 457.13 | J/mol×K | 790.29 | 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=U292582&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 |