# 2,6-Difluorobenzoic acid, hex-4-yn-3-yl ester

**Inchi:** InChI=1S/C13H12F2O2/c1-3-6-9(4-2)17-13(16)12-10(14)7-5-8-11(12)15/h5,7-9H,4H2,1-
**InchiKey:** MRLUKPZMKZZDKY-UHFFFAOYSA-N
**Formula:** C13H12F2O2
**SMILES:** CC#CC(CC)OC(=O)c1c(F)cccc1F
**Mol. weight [g/mol]:** 238.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -271.45 | kJ/mol | Joback Method |
| hf | -468.06 | kJ/mol | Joback Method |
| hfus | 31.24 | kJ/mol | Joback Method |
| hvap | 57.42 | kJ/mol | Joback Method |
| log10ws | -4.38 | | Crippen Method |
| logp | 2.923 | | Crippen Method |
| mcvol | 172.650 | ml/mol | McGowan Method |
| pc | 2400.57 | kPa | Joback Method |
| rinpol | 1549.50 | | NIST Webbook |
| rinpol | 1549.50 | | NIST Webbook |
| tb | 616.87 | K | Joback Method |
| tc | 829.53 | K | Joback Method |
| tf | 452.17 | K | Joback Method |
| vc | 0.671 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 418.72 | J/mol×K | 616.87 | Joback Method |
| cpg | 432.30 | J/mol×K | 652.31 | Joback Method |
| cpg | 445.10 | J/mol×K | 687.76 | Joback Method |
| cpg | 457.14 | J/mol×K | 723.20 | Joback Method |
| cpg | 468.44 | J/mol×K | 758.64 | Joback Method |
| cpg | 479.01 | J/mol×K | 794.09 | Joback Method |
| cpg | 488.85 | J/mol×K | 829.53 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U292584&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 |

# 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 |