# «beta»-Alanine, N-(2,6-difluorobenzoyl)-, propyl ester

**Inchi:** InChI=1S/C13H15F2NO3/c1-2-8-19-11(17)6-7-16-13(18)12-9(14)4-3-5-10(12)15/h3-5H,2

**InchiKey:** CFMOGIPGQWTXEY-UHFFFAOYSA-N

**Formula:** C13H15F2NO3

**SMILES:** CCCOC(=O)CCNC(=O)c1c(F)cccc1F

**Mol. weight [g/mol]:** 271.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -511.34 | kJ/mol | Joback Method |
| hf | -794.19 | kJ/mol | Joback Method |
| hfus | 38.33 | kJ/mol | Joback Method |
| hvap | 68.84 | kJ/mol | Joback Method |
| log10ws | -3.43 | | Crippen Method |
| logp | 2.038 | | Crippen Method |
| mcvol | 192.800 | ml/mol | McGowan Method |
| pc | 2197.95 | kPa | Joback Method |
| rinpol | 1972.00 | | NIST Webbook |
| tb | 712.35 | K | Joback Method |
| tc | 908.47 | K | Joback Method |
| tf | 463.66 | K | Joback Method |
| vc | 0.756 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 528.64 | J/mol×K | 712.35 | Joback Method |
| cpg | 541.11 | J/mol×K | 745.04 | Joback Method |
| cpg | 552.81 | J/mol×K | 777.72 | Joback Method |
| cpg | 563.75 | J/mol×K | 810.41 | Joback Method |
| cpg | 573.94 | J/mol×K | 843.10 | Joback Method |
| cpg | 583.41 | J/mol×K | 875.79 | Joback Method |
| cpg | 592.16 | J/mol×K | 908.47 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321840&Units=SI |

# 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 |