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

**Inchi:** InChI=1S/C21H31F2NO3/c1-2-3-4-5-6-7-8-9-10-16-27-19(25)14-15-24-21(26)20-17(22)1
**InchiKey:** ULDHCRXNENUWRS-UHFFFAOYSA-N
**Formula:** C21H31F2NO3
**SMILES:** CCCCCCCCCCCOC(=O)CCNC(=O)c1c(F)cccc1F
**Mol. weight [g/mol]:** 383.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -443.98 | kJ/mol | Joback Method |
| hf | -959.31 | kJ/mol | Joback Method |
| hfus | 59.05 | kJ/mol | Joback Method |
| hvap | 86.64 | kJ/mol | Joback Method |
| log10ws | -6.78 | | Crippen Method |
| logp | 5.159 | | Crippen Method |
| mcvol | 305.520 | ml/mol | McGowan Method |
| pc | 1188.24 | kPa | Joback Method |
| rinpol | 2807.00 | | NIST Webbook |
| rinpol | 2807.00 | | NIST Webbook |
| tb | 895.39 | K | Joback Method |
| tc | 1097.39 | K | Joback Method |
| tf | 553.82 | K | Joback Method |
| vc | 1.204 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 981.39 | J/mol×K | 895.39 | Joback Method |
| cpg | 996.82 | J/mol×K | 929.06 | Joback Method |
| cpg | 1011.12 | J/mol×K | 962.72 | Joback Method |
| cpg | 1024.35 | J/mol×K | 996.39 | Joback Method |
| cpg | 1036.52 | J/mol×K | 1030.05 | Joback Method |
| cpg | 1047.69 | J/mol×K | 1063.72 | Joback Method |
| cpg | 1057.90 | J/mol×K | 1097.39 | Joback Method |

# Sources

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|---|---|
| **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=U321849&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 |