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

**Inchi:** InChI=1S/C24H37F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-30-22(28)17-18-27-24(29)2

**InchiKey:** OOQPBINVCQVNML-UHFFFAOYSA-N

**Formula:** C24H37F2NO3

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

**Mol. weight [g/mol]:** 425.55

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -418.72 | kJ/mol | Joback Method |
| hf | -1021.23 | kJ/mol | Joback Method |
| hfus | 66.82 | kJ/mol | Joback Method |
| hvap | 93.32 | kJ/mol | Joback Method |
| log10ws | -8.04 | | Crippen Method |
| logp | 6.329 | | Crippen Method |
| mcvol | 347.790 | ml/mol | McGowan Method |
| pc | 983.31 | kPa | Joback Method |
| rinpol | 3317.00 | | NIST Webbook |
| rinpol | 3317.00 | | NIST Webbook |
| tb | 964.03 | K | Joback Method |
| tc | 1181.31 | K | Joback Method |
| tf | 587.63 | K | Joback Method |
| vc | 1.373 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1163.99 | J/mol×K | 964.03 | Joback Method |
| cpg | 1180.58 | J/mol×K | 1000.24 | Joback Method |
| cpg | 1195.82 | J/mol×K | 1036.46 | Joback Method |
| cpg | 1209.76 | J/mol×K | 1072.67 | Joback Method |
| cpg | 1222.47 | J/mol×K | 1108.88 | Joback Method |
| cpg | 1234.00 | J/mol×K | 1145.09 | Joback Method |
| cpg | 1244.40 | J/mol×K | 1181.31 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321851&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

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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 |