# «beta»-Alanine, N-(4-trifluoromethylbenzoyl)-, dodecyl ester

**Inchi:** InChI=1S/C23H34F3NO3/c1-2-3-4-5-6-7-8-9-10-11-18-30-21(28)16-17-27-22(29)19-12-1

**InchiKey:** FUYMHALPBGXRCY-UHFFFAOYSA-N

**Formula:** C23H34F3NO3

**SMILES:** CCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(C(F)(F)F)cc1

**Mol. weight [g/mol]:** 429.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -609.48 | kJ/mol | Joback Method |
| hf | -1193.98 | kJ/mol | Joback Method |
| hfus | 60.29 | kJ/mol | Joback Method |
| hvap | 88.32 | kJ/mol | Joback Method |
| log10ws | -7.64 | | Crippen Method |
| logp | 6.289 | | Crippen Method |
| mcvol | 335.470 | ml/mol | McGowan Method |
| pc | 1037.90 | kPa | Joback Method |
| rinpol | 2844.00 | | NIST Webbook |
| rinpol | 2844.00 | | NIST Webbook |
| tb | 932.21 | K | Joback Method |
| tc | 1141.29 | K | Joback Method |
| tf | 566.85 | K | Joback Method |
| vc | 1.323 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1110.44 | J/mol×K | 932.21 | Joback Method |
| cpg | 1126.42 | J/mol×K | 967.06 | Joback Method |
| cpg | 1141.24 | J/mol×K | 1001.90 | Joback Method |
| cpg | 1154.99 | J/mol×K | 1036.75 | Joback Method |
| cpg | 1167.74 | J/mol×K | 1071.60 | Joback Method |
| cpg | 1179.56 | J/mol×K | 1106.44 | Joback Method |
| cpg | 1190.53 | J/mol×K | 1141.29 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321746&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 |