# «beta»-Alanine, N-(3-trifluoromethylbenzoyl)-, decyl ester

**Inchi:** InChI=1S/C21H30F3NO3/c1-2-3-4-5-6-7-8-9-15-28-19(26)13-14-25-20(27)17-11-10-12-1

**InchiKey:** SLTRGONNPNBSKM-UHFFFAOYSA-N

**Formula:** C21H30F3NO3

**SMILES:** CCCCCCCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1

**Mol. weight [g/mol]:** 401.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -626.32 | kJ/mol | Joback Method |
| hf | -1152.70 | kJ/mol | Joback Method |
| hfus | 55.11 | kJ/mol | Joback Method |
| hvap | 83.87 | kJ/mol | Joback Method |
| log10ws | -6.81 | | Crippen Method |
| logp | 5.509 | | Crippen Method |
| mcvol | 307.290 | ml/mol | McGowan Method |
| pc | 1179.28 | kPa | Joback Method |
| rinpol | 2634.00 | | NIST Webbook |
| tb | 886.45 | K | Joback Method |
| tc | 1087.07 | K | Joback Method |
| tf | 544.31 | K | Joback Method |
| vc | 1.212 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 989.91 | J/mol×K | 886.45 | Joback Method |
| cpg | 1005.08 | J/mol×K | 919.89 | Joback Method |
| cpg | 1019.21 | J/mol×K | 953.32 | Joback Method |
| cpg | 1032.34 | J/mol×K | 986.76 | Joback Method |
| cpg | 1044.54 | J/mol×K | 1020.19 | Joback Method |
| cpg | 1055.86 | J/mol×K | 1053.63 | Joback Method |
| cpg | 1066.37 | J/mol×K | 1087.07 | 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=U321593&Units=SI |

# 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 |