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

**Inchi:** InChI=1S/C27H42F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-34-25(32)20-21-31-2

**InchiKey:** XXWMNUOYDQEQSB-UHFFFAOYSA-N

**Formula:** C27H42F3NO3

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

**Mol. weight [g/mol]:** 485.62

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -575.80 | kJ/mol | Joback Method |
| hf | -1276.54 | kJ/mol | Joback Method |
| hfus | 70.65 | kJ/mol | Joback Method |
| hvap | 97.22 | kJ/mol | Joback Method |
| log10ws | -9.32 | | Crippen Method |
| logp | 7.850 | | Crippen Method |
| mcvol | 391.830 | ml/mol | McGowan Method |
| pc | 821.95 | kPa | Joback Method |
| tb | 1023.73 | K | Joback Method |
| tc | 1262.40 | K | Joback Method |
| tf | 611.93 | K | Joback Method |
| vc | 1.548 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1358.38 | J/mol×K | 1023.73 | Joback Method |
| cpg | 1376.51 | J/mol×K | 1063.51 | Joback Method |
| cpg | 1393.19 | J/mol×K | 1103.29 | Joback Method |
| cpg | 1408.57 | J/mol×K | 1143.07 | Joback Method |
| cpg | 1422.76 | J/mol×K | 1182.84 | Joback Method |
| cpg | 1435.89 | J/mol×K | 1222.62 | Joback Method |
| cpg | 1448.09 | J/mol×K | 1262.40 | Joback Method |

# Sources

| | |
|---|---|
| **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=U321749&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |