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

**Inchi:** InChI=1S/C17H22F3NO3/c1-2-3-4-5-12-24-15(22)10-11-21-16(23)13-6-8-14(9-7-13)17(1

**InchiKey:** PHBHSMVQPXUMRW-UHFFFAOYSA-N

**Formula:** C17H22F3NO3

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

**Mol. weight [g/mol]:** 345.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -660.00 | kJ/mol | Joback Method |
| hf | -1070.14 | kJ/mol | Joback Method |
| hfus | 44.75 | kJ/mol | Joback Method |
| hvap | 74.97 | kJ/mol | Joback Method |
| log10ws | -5.13 | | Crippen Method |
| logp | 3.949 | | Crippen Method |
| mcvol | 250.930 | ml/mol | McGowan Method |
| pc | 1564.75 | kPa | Joback Method |
| rinpol | 2210.00 | | NIST Webbook |
| tb | 794.93 | K | Joback Method |
| tc | 988.51 | K | Joback Method |
| tf | 499.23 | K | Joback Method |
| vc | 0.988 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 757.65 | J/mol×K | 794.93 | Joback Method |
| cpg | 771.49 | J/mol×K | 827.19 | Joback Method |
| cpg | 784.40 | J/mol×K | 859.46 | Joback Method |
| cpg | 796.43 | J/mol×K | 891.72 | Joback Method |
| cpg | 807.62 | J/mol×K | 923.98 | Joback Method |
| cpg | 818.01 | J/mol×K | 956.24 | Joback Method |
| cpg | 827.66 | J/mol×K | 988.51 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321740&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 |