# «beta»-Alanine, N-(3-methylbenzoyl)-, isohexyl ester

**Inchi:** InChI=1S/C17H25NO3/c1-13(2)6-5-11-21-16(19)9-10-18-17(20)15-8-4-7-14(3)12-15/h4,7

**InchiKey:** FFFIGCZGYBFMAM-UHFFFAOYSA-N

**Formula:** C17H25NO3

**SMILES:** Cc1cccc(C(=O)NCCC(=O)OCCCC(C)C)c1

**Mol. weight [g/mol]:** 291.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -80.85 | kJ/mol | Joback Method |
| hf | -478.34 | kJ/mol | Joback Method |
| hfus | 39.40 | kJ/mol | Joback Method |
| hvap | 78.32 | kJ/mol | Joback Method |
| log10ws | -4.26 | | Crippen Method |
| logp | 3.094 | | Crippen Method |
| mcvol | 245.620 | ml/mol | McGowan Method |
| pc | 1730.34 | kPa | Joback Method |
| rinpol | 2369.00 | | NIST Webbook |
| rinpol | 2369.00 | | NIST Webbook |
| tb | 799.91 | K | Joback Method |
| tc | 1005.41 | K | Joback Method |
| tf | 480.04 | K | Joback Method |
| vc | 0.939 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 733.88 | J/mol×K | 799.91 | Joback Method |
| cpg | 749.14 | J/mol×K | 834.16 | Joback Method |
| cpg | 763.35 | J/mol×K | 868.41 | Joback Method |
| cpg | 776.54 | J/mol×K | 902.66 | Joback Method |
| cpg | 788.75 | J/mol×K | 936.91 | Joback Method |
| cpg | 800.01 | J/mol×K | 971.16 | Joback Method |
| cpg | 810.35 | J/mol×K | 1005.41 | 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=U321628&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |

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