

«beta»-Alanine, N-isobutyryl-, decyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C17H33NO3/c1-4-5-6-7-8-9-10-11-14-21-16(19)12-13-18-17(20)15(2)3/h15H,4 |
| InchiKey: | FZRIUIAKXRPAQS-UHFFFAOYSA-N |
| Formula: | C17H33NO3 |
| SMILES: | CCCCCCCCCOC(=O)CCNC(=O)C(C)C |
| Mol. weight [g/mol]: | 299.45 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -183.63 | kJ/mol | Joback Method |
| hf | -703.40 | kJ/mol | Joback Method |
| hfus | 45.75 | kJ/mol | Joback Method |
| hvap | 75.39 | kJ/mol | Joback Method |
| log10ws | -4.52 | | Crippen Method |
| logp | 3.833 | | Crippen Method |
| mcvol | 269.380 | ml/mol | McGowan Method |
| pc | 1351.64 | kPa | Joback Method |
| rinpol | 2208.00 | | NIST Webbook |
| rinpol | 2208.00 | | NIST Webbook |
| tb | 768.25 | K | Joback Method |
| tc | 950.75 | K | Joback Method |
| tf | 441.10 | K | Joback Method |
| vc | 1.046 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 823.32 | J/mol×K | 768.25 | Joback Method |
| cpg | 840.28 | J/mol×K | 798.67 | Joback Method |
| cpg | 856.32 | J/mol×K | 829.08 | Joback Method |
| cpg | 871.45 | J/mol×K | 859.50 | Joback Method |
| cpg | 885.72 | J/mol×K | 889.92 | Joback Method |
| cpg | 899.12 | J/mol×K | 920.33 | Joback Method |
| cpg | 911.70 | J/mol×K | 950.75 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U321668&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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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