# «beta»-Alanine, N-(1-naphthoyl)-, ethyl ester

**Inchi:** InChI=1S/C16H17NO3/c1-2-20-15(18)10-11-17-16(19)14-9-5-7-12-6-3-4-8-13(12)14/h3-9
**InchiKey:** SLYQVPOOQAIFIQ-UHFFFAOYSA-N
**Formula:** C16H17NO3
**SMILES:** CCOC(=O)CCNC(=O)c1cccc2ccccc12
**Mol. weight [g/mol]:** 271.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 19.82 | kJ/mol | Joback Method |
| hf | -261.35 | kJ/mol | Joback Method |
| hfus | 37.35 | kJ/mol | Joback Method |
| hvap | 78.13 | kJ/mol | Joback Method |
| log10ws | -4.16 | | Crippen Method |
| logp | 2.523 | | Crippen Method |
| mcvol | 212.070 | ml/mol | McGowan Method |
| pc | 2331.52 | kPa | Joback Method |
| rinpol | 2448.00 | | NIST Webbook |
| rinpol | 2448.00 | | NIST Webbook |
| tb | 796.45 | K | Joback Method |
| tc | 1019.72 | K | Joback Method |
| tf | 516.47 | K | Joback Method |
| vc | 0.810 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 605.11 | J/mol×K | 796.45 | Joback Method |
| cpg | 618.23 | J/mol×K | 833.66 | Joback Method |
| cpg | 630.38 | J/mol×K | 870.87 | Joback Method |
| cpg | 641.62 | J/mol×K | 908.09 | Joback Method |
| cpg | 652.01 | J/mol×K | 945.30 | Joback Method |
| cpg | 661.61 | J/mol×K | 982.51 | Joback Method |
| cpg | 670.48 | J/mol×K | 1019.72 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321944&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 |