# L-Norvaline, N-(but-2-yn-1-yloxycarbonyl)-, heptyl ester

**Inchi:** InChI=1S/C17H29NO4/c1-4-7-9-10-11-14-21-16(19)15(12-6-3)18-17(20)22-13-8-5-2/h15

**InchiKey:** ZIVBYWDOSCWFRS-OAHLLOKOSA-N

**Formula:** C17H29NO4

**SMILES:** CC#CCOC(=O)NC(CCC)C(=O)OCCCCCCC

**Mol. weight [g/mol]:** 311.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -85.83 | kJ/mol | Joback Method |
| hf | -563.32 | kJ/mol | Joback Method |
| hfus | 50.06 | kJ/mol | Joback Method |
| hvap | 79.95 | kJ/mol | Joback Method |
| log10ws | -4.74 | | Crippen Method |
| logp | 3.418 | | Crippen Method |
| mcvol | 266.650 | ml/mol | McGowan Method |
| pc | 1505.81 | kPa | Joback Method |
| rinpol | 2199.00 | | NIST Webbook |
| rinpol | 2199.00 | | NIST Webbook |
| tb | 799.67 | K | Joback Method |
| tc | 993.90 | K | Joback Method |
| tf | 569.43 | K | Joback Method |
| vc | 1.026 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 804.68 | J/mol×K | 799.67 | Joback Method |
| cpg | 820.62 | J/mol×K | 832.04 | Joback Method |
| cpg | 835.57 | J/mol×K | 864.41 | Joback Method |
| cpg | 849.55 | J/mol×K | 896.79 | Joback Method |
| cpg | 862.56 | J/mol×K | 929.16 | Joback Method |
| cpg | 874.62 | J/mol×K | 961.53 | Joback Method |
| cpg | 885.73 | J/mol×K | 993.90 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392864&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |