# l-Norvaline, n-butoxycarbonyl-, octadecyl ester

**Inchi:** InChI=1S/C28H55NO4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-32-27(30)2

**InchiKey:** XWXWNUJKLZFDGT-UHFFFAOYSA-N

**Formula:** C28H55NO4

**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCCCC

**Mol. weight [g/mol]:** 469.74

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -196.01 | kJ/mol | Joback Method |
| hf | -1062.66 | kJ/mol | Joback Method |
| hfus | 75.43 | kJ/mol | Joback Method |
| hvap | 102.28 | kJ/mol | Joback Method |
| log10ws | -9.55 | | Crippen Method |
| logp | 8.486 | | Crippen Method |
| mcvol | 430.240 | ml/mol | McGowan Method |
| pc | 695.08 | kPa | Joback Method |
| tb | 1042.35 | K | Joback Method |
| tc | 1303.56 | K | Joback Method |
| tf | 587.30 | K | Joback Method |
| vc | 1.681 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1540.25 | J/mol×K | 1042.35 | Joback Method |
| cpg | 1562.39 | J/mol×K | 1085.88 | Joback Method |
| cpg | 1582.15 | J/mol×K | 1129.42 | Joback Method |
| cpg | 1599.64 | J/mol×K | 1172.95 | Joback Method |
| cpg | 1614.96 | J/mol×K | 1216.49 | Joback Method |
| cpg | 1628.21 | J/mol×K | 1260.02 | Joback Method |
| cpg | 1639.49 | J/mol×K | 1303.56 | Joback Method |

# Sources

| | |
|---|---|
| **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=U320784&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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