# L-Norvaline, N-allyloxycarbonyl-, hexadecyl ester

**Inchi:** InChI=1S/C25H47NO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-29-24(27)23(20-5-

**InchiKey:** UWNRTXWFUVNINM-UHFFFAOYSA-N

**Formula:** C25H47NO4

**SMILES:** C=CCOC(=O)NC(CCC)C(=O)OCCCCCCCCCCCCCCCC

**Mol. weight [g/mol]:** 425.65

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 66.38 | kJ/mol | Joback Method |
| log10ws | -6.91 | | Cheméo Relay (1.0) |
| logp | 7.092 | | Crippen Method |
| mcvol | 383.670 | ml/mol | McGowan Method |
| rinpol | 2585.00 | | NIST Webbook |
| rinpol | 2585.00 | | NIST Webbook |
| tb | 663.54 | K | Cheméo Relay (1.0) |
| tf | 315.36 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1317.33 | J/mol×K | 970.39 | Joback Method |
| cpg | 1336.98 | J/mol×K | 1007.71 | Joback Method |
| cpg | 1355.00 | J/mol×K | 1045.03 | Joback Method |
| cpg | 1371.43 | J/mol×K | 1082.36 | Joback Method |
| cpg | 1386.34 | J/mol×K | 1119.68 | Joback Method |
| cpg | 1399.79 | J/mol×K | 1157.00 | Joback Method |
| cpg | 1411.82 | J/mol×K | 1194.32 | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U320755&Units=SI

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |