# l-Norvaline, N-allyloxycarbonyl-, isohexyl ester

**Inchi:** InChI=1S/C15H27NO4/c1-5-8-13(16-15(18)20-10-6-2)14(17)19-11-7-9-12(3)4/h6,12-13H

**InchiKey:** JISMMAQOALHKMT-UHFFFAOYSA-N

**Formula:** C15H27NO4

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

**Mol. weight [g/mol]:** 285.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -694.88 | kJ/mol | Joback Method |
| hvap | 79.18 | kJ/mol | Joback Method |
| log10ws | -3.25 | | Crippen Method |
| logp | 3.251 | | Crippen Method |
| mcvol | 242.770 | ml/mol | McGowan Method |
| pc | 1503.48 | kPa | Joback Method |
| rinpol | 1709.00 | | NIST Webbook |
| tb | 805.85 | K | Joback Method |
| tc | 995.79 | K | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U320746&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

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

## Legend

**hf:** Enthalpy of formation 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 |