# L-Valine, N-(3-methylbut-2-enoyl)-, octyl ester

**Inchi:** InChI=1S/C18H33NO3/c1-6-7-8-9-10-11-12-22-18(21)17(15(4)5)19-16(20)13-14(2)3/h13
**InchiKey:** JWGONWAWBPYNBZ-UHFFFAOYSA-N
**Formula:** C18H33NO3
**SMILES:** CCCCCCCCOC(=O)C(N=C(O)C=C(C)C)C(C)C
**Mol. weight [g/mol]:** 311.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -642.58 | kJ/mol | Joback Method |
| hvap | 84.15 | kJ/mol | Joback Method |
| log10ws | -4.93 | | Crippen Method |
| logp | 4.837 | | Crippen Method |
| mcvol | 279.170 | ml/mol | McGowan Method |
| pc | 1244.21 | kPa | Joback Method |
| rinpol | 2179.00 | | NIST Webbook |
| rinpol | 2179.00 | | NIST Webbook |
| tb | 859.43 | K | Joback Method |
| tc | 1056.27 | K | Joback Method |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U346072&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

**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 |