# DL-Valine, N-methyl-N-octyloxycarbonyl-, butyl ester

**Inchi:** InChI=1S/C19H37NO4/c1-6-8-10-11-12-13-15-24-19(22)20(5)17(16(3)4)18(21)23-14-9-7

**InchiKey:** FHYFFGWGOVKLII-UHFFFAOYSA-N

**Formula:** C19H37NO4

**SMILES:** CCCCCCCCOC(=O)N(C)C(C(=O)OCCCC)C(C)C

**Mol. weight [g/mol]:** 343.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -252.84 | kJ/mol | Joback Method |
| hf | -868.12 | kJ/mol | Joback Method |
| hfus | 46.52 | kJ/mol | Joback Method |
| hvap | 77.47 | kJ/mol | Joback Method |
| log10ws | -4.92 | | Crippen Method |
| logp | 4.783 | | Crippen Method |
| mcvol | 303.430 | ml/mol | McGowan Method |
| pc | 1160.08 | kPa | Joback Method |
| rinpol | 2143.00 | | NIST Webbook |
| rinpol | 2143.00 | | NIST Webbook |
| tb | 798.26 | K | Joback Method |
| tc | 982.17 | K | Joback Method |
| tf | 450.68 | K | Joback Method |
| vc | 1.153 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 952.86 | J/mol×K | 798.26 | Joback Method |
| cpg | 971.04 | J/mol×K | 828.91 | Joback Method |
| cpg | 988.16 | J/mol×K | 859.56 | Joback Method |
| cpg | 1004.24 | J/mol×K | 890.22 | Joback Method |
| cpg | 1019.32 | J/mol×K | 920.87 | Joback Method |
| cpg | 1033.40 | J/mol×K | 951.52 | Joback Method |
| cpg | 1046.51 | J/mol×K | 982.17 | Joback Method |

# Sources

| | |
|---|---|
| **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=U392900&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |