# DL-Valine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, 2-ethylhexyl ester

**Inchi:** InChI=1S/C23H45NO4/c1-8-12-14-19(10-3)16-27-22(25)21(18(5)6)24(7)23(26)28-17-20(
**InchiKey:** HAPMECDFNLCJQM-UHFFFAOYSA-N
**Formula:** C23H45NO4
**SMILES:** CCCCC(CC)COC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC
**Mol. weight [g/mol]:** 399.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -224.04 | kJ/mol | Joback Method |
| hf | -961.24 | kJ/mol | Joback Method |
| hfus | 49.83 | kJ/mol | Joback Method |
| hvap | 85.59 | kJ/mol | Joback Method |
| log10ws | -6.11 | | Crippen Method |
| logp | 6.055 | | Crippen Method |
| mcvol | 359.790 | ml/mol | McGowan Method |
| pc | 916.05 | kPa | Joback Method |
| rinpol | 2329.00 | | NIST Webbook |
| rinpol | 2329.00 | | NIST Webbook |
| tb | 888.90 | K | Joback Method |
| tc | 1088.27 | K | Joback Method |
| tf | 465.76 | K | Joback Method |
| vc | 1.365 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1200.62 | J/mol×K | 888.90 | Joback Method |
| cpg | 1220.31 | J/mol×K | 922.13 | Joback Method |
| cpg | 1238.63 | J/mol×K | 955.36 | Joback Method |
| cpg | 1255.61 | J/mol×K | 988.59 | Joback Method |
| cpg | 1271.29 | J/mol×K | 1021.82 | Joback Method |
| cpg | 1285.71 | J/mol×K | 1055.04 | Joback Method |
| cpg | 1298.90 | J/mol×K | 1088.27 | Joback Method |

# Sources

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|---|---|
| **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=U392923&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |