# L-Valine, N-(3-bromobenzoyl)-, pentadecyl ester

**Inchi:** InChI=1S/C27H44BrNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-32-27(31)25(22(2)3)2

**InchiKey:** GYPIFIWVOUPVMD-UHFFFAOYSA-N

**Formula:** C27H44BrNO3

**SMILES:** CCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C

**Mol. weight [g/mol]:** 510.55

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 15.23 | kJ/mol | Joback Method |
| hf | -663.69 | kJ/mol | Joback Method |
| hfus | 67.06 | kJ/mol | Joback Method |
| hvap | 106.63 | kJ/mol | Joback Method |
| log10ws | -9.67 | | Crippen Method |
| logp | 7.838 | | Crippen Method |
| mcvol | 404.020 | ml/mol | McGowan Method |
| pc | 925.55 | kPa | Joback Method |
| rinpol | 3470.00 | | NIST Webbook |
| tb | 1094.43 | K | Joback Method |
| tc | 1344.73 | K | Joback Method |
| tf | 637.54 | K | Joback Method |
| vc | 1.554 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1377.60 | J/mol×K | 1094.43 | Joback Method |
| cpg | 1394.02 | J/mol×K | 1136.15 | Joback Method |
| cpg | 1408.95 | J/mol×K | 1177.86 | Joback Method |
| cpg | 1422.51 | J/mol×K | 1219.58 | Joback Method |
| cpg | 1434.83 | J/mol×K | 1261.29 | Joback Method |
| cpg | 1446.02 | J/mol×K | 1303.01 | Joback Method |
| cpg | 1456.22 | J/mol×K | 1344.73 | Joback Method |

# Sources

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|---|---|
| **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=U346696&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 |