# L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, heptadecyl ester

**Inchi:** InChI=1S/C31H47F6NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-41-29(40)27(23

**InchiKey:** LASHZNQDFNMKKY-UHFFFAOYSA-N

**Formula:** C31H47F6NO3

**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

**Mol. weight [g/mol]:** 595.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1138.22 | kJ/mol | Joback Method |
| hf | -1978.21 | kJ/mol | Joback Method |
| hfus | 75.40 | kJ/mol | Joback Method |
| hvap | 102.27 | kJ/mol | Joback Method |
| log10ws | -11.55 | | Crippen Method |
| logp | 9.893 | | Crippen Method |
| mcvol | 453.500 | ml/mol | McGowan Method |
| pc | 629.08 | kPa | Joback Method |
| rinpol | 3163.00 | | NIST Webbook |
| rinpol | 3163.00 | | NIST Webbook |
| tb | 1113.93 | K | Joback Method |
| tc | 1410.67 | K | Joback Method |
| tf | 643.72 | K | Joback Method |
| vc | 1.802 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1631.91 | J/mol×K | 1113.93 | Joback Method |
| cpg | 1653.51 | J/mol×K | 1163.39 | Joback Method |
| cpg | 1673.42 | J/mol×K | 1212.84 | Joback Method |
| cpg | 1691.96 | J/mol×K | 1262.30 | Joback Method |
| cpg | 1709.46 | J/mol×K | 1311.76 | Joback Method |
| cpg | 1726.23 | J/mol×K | 1361.21 | Joback Method |
| cpg | 1742.60 | J/mol×K | 1410.67 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U346581&Units=SI |

# 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 |