# L-Valine, N-pentafluorobenzoyl-, heptadecyl ester

**Inchi:** InChI=1S/C29H44F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-38-29(37)27(20

**InchiKey:** HXVCZIYSLVGVQX-UHFFFAOYSA-N

**Formula:** C29H44F5NO3

**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C

**Mol. weight [g/mol]:** 549.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -994.82 | kJ/mol | Joback Method |
| hf | -1757.73 | kJ/mol | Joback Method |
| hfus | 80.80 | kJ/mol | Joback Method |
| hvap | 103.21 | kJ/mol | Joback Method |
| log10ws | -11.00 | | Crippen Method |
| logp | 8.551 | | Crippen Method |
| mcvol | 423.550 | ml/mol | McGowan Method |
| pc | 680.65 | kPa | Joback Method |
| rinpol | 3208.00 | | NIST Webbook |
| rinpol | 3208.00 | | NIST Webbook |
| tb | 1090.30 | K | Joback Method |
| tc | 1377.25 | K | Joback Method |
| tf | 653.31 | K | Joback Method |
| vc | 1.694 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1494.57 | J/mol×K | 1090.30 | Joback Method |
| cpg | 1513.40 | J/mol×K | 1138.12 | Joback Method |
| cpg | 1529.68 | J/mol×K | 1185.95 | Joback Method |
| cpg | 1543.55 | J/mol×K | 1233.77 | Joback Method |
| cpg | 1555.13 | J/mol×K | 1281.60 | Joback Method |
| cpg | 1564.55 | J/mol×K | 1329.42 | Joback Method |
| cpg | 1571.95 | J/mol×K | 1377.25 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U346616&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

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