# L-Valine, N-(3,4-difluorobenzoyl)-, tetradecyl ester

**Inchi:** InChI=1S/C26H41F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-32-26(31)24(20(2)3)29-2

**InchiKey:** FKZKMDCAYMPRGE-UHFFFAOYSA-N

**Formula:** C26H41F2NO3

**SMILES:** CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)c(F)c1)C(C)C

**Mol. weight [g/mol]:** 453.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -406.76 | kJ/mol | Joback Method |
| hf | -1073.07 | kJ/mol | Joback Method |
| hfus | 64.96 | kJ/mol | Joback Method |
| hvap | 97.00 | kJ/mol | Joback Method |
| log10ws | -8.75 | | Crippen Method |
| logp | 6.964 | | Crippen Method |
| mcvol | 375.970 | ml/mol | McGowan Method |
| pc | 883.14 | kPa | Joback Method |
| rinpol | 3026.00 | | NIST Webbook |
| rinpol | 3026.00 | | NIST Webbook |
| tb | 1008.91 | K | Joback Method |
| tc | 1239.03 | K | Joback Method |
| tf | 580.17 | K | Joback Method |
| vc | 1.472 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1288.96 | J/mol×K | 1008.91 | Joback Method |
| cpg | 1306.15 | J/mol×K | 1047.26 | Joback Method |
| cpg | 1321.79 | J/mol×K | 1085.62 | Joback Method |
| cpg | 1335.93 | J/mol×K | 1123.97 | Joback Method |
| cpg | 1348.67 | J/mol×K | 1162.32 | Joback Method |
| cpg | 1360.07 | J/mol×K | 1200.67 | Joback Method |
| cpg | 1370.21 | J/mol×K | 1239.03 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U346510&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 |