# L-Valine, N-(3-chloro-2-fluorobenzoyl)-, undecyl ester

**Inchi:** InChI=1S/C23H35ClFNO3/c1-4-5-6-7-8-9-10-11-12-16-29-23(28)21(17(2)3)26-22(27)18-

**InchiKey:** IWDFXPNAANJEFZ-UHFFFAOYSA-N

**Formula:** C23H35ClFNO3

**SMILES:** CCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(Cl)c1F)C(C)C

**Mol. weight [g/mol]:** 427.98

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -249.14 | kJ/mol | Joback Method |
| hf | -830.78 | kJ/mol | Joback Method |
| hfus | 58.30 | kJ/mol | Joback Method |
| hvap | 95.52 | kJ/mol | Joback Method |
| log10ws | -7.84 | | Crippen Method |
| logp | 6.308 | | Crippen Method |
| mcvol | 344.170 | ml/mol | McGowan Method |
| pc | 1061.71 | kPa | Joback Method |
| rinpol | 2922.00 | | NIST Webbook |
| rinpol | 2922.00 | | NIST Webbook |
| tb | 978.43 | K | Joback Method |
| tc | 1197.94 | K | Joback Method |
| tf | 575.69 | K | Joback Method |
| vc | 1.335 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1122.07 | J/mol×K | 978.43 | Joback Method |
| cpg | 1137.22 | J/mol×K | 1015.02 | Joback Method |
| cpg | 1151.05 | J/mol×K | 1051.60 | Joback Method |
| cpg | 1163.63 | J/mol×K | 1088.19 | Joback Method |
| cpg | 1175.00 | J/mol×K | 1124.77 | Joback Method |
| cpg | 1185.23 | J/mol×K | 1161.36 | Joback Method |
| cpg | 1194.36 | J/mol×K | 1197.94 | Joback Method |

# Sources

| | |
|---|---|
| **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=U346545&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |

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