# L-Valine, N-(4-fluorobenzoyl)-, octyl ester

**Inchi:** InChI=1S/C20H30FNO3/c1-4-5-6-7-8-9-14-25-20(24)18(15(2)3)22-19(23)16-10-12-17(21
**InchiKey:** OAQJXTOVVWZRMA-UHFFFAOYSA-N
**Formula:** C20H30FNO3
**SMILES:** CCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
**Mol. weight [g/mol]:** 351.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -252.84 | kJ/mol | Joback Method |
| hf | -741.65 | kJ/mol | Joback Method |
| hfus | 46.73 | kJ/mol | Joback Method |
| hvap | 83.80 | kJ/mol | Joback Method |
| log10ws | -5.90 | | Crippen Method |
| logp | 4.484 | | Crippen Method |
| mcvol | 289.660 | ml/mol | McGowan Method |
| pc | 1342.74 | kPa | Joback Method |
| rinpol | 2442.00 | | NIST Webbook |
| rinpol | 2442.00 | | NIST Webbook |
| tb | 867.38 | K | Joback Method |
| tc | 1070.37 | K | Joback Method |
| tf | 499.44 | K | Joback Method |
| vc | 1.119 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 916.27 | J/mol×K | 867.38 | Joback Method |
| cpg | 931.88 | J/mol×K | 901.21 | Joback Method |
| cpg | 946.37 | J/mol×K | 935.04 | Joback Method |
| cpg | 959.76 | J/mol×K | 968.87 | Joback Method |
| cpg | 972.11 | J/mol×K | 1002.70 | Joback Method |
| cpg | 983.44 | J/mol×K | 1036.54 | Joback Method |
| cpg | 993.81 | J/mol×K | 1070.37 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U346668&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

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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 |