# L-Valine, N-(5-fluoro-2-trifluoromethyl)-, pentyl ester

**Inchi:** InChI=1S/C18H23F4NO3/c1-4-5-6-9-26-17(25)15(11(2)3)23-16(24)13-10-12(19)7-8-14(1

**InchiKey:** AFLJIOVWFKRJEF-UHFFFAOYSA-N

**Formula:** C18H23F4NO3

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

**Mol. weight [g/mol]:** 377.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -860.90 | kJ/mol | Joback Method |
| hf | -1308.92 | kJ/mol | Joback Method |
| hfus | 42.98 | kJ/mol | Joback Method |
| hvap | 76.26 | kJ/mol | Joback Method |
| log10ws | -5.75 | | Crippen Method |
| logp | 4.332 | | Crippen Method |
| mcvol | 266.790 | ml/mol | McGowan Method |
| pc | 1404.84 | kPa | Joback Method |
| rinpol | 2055.00 | | NIST Webbook |
| rinpol | 2055.00 | | NIST Webbook |
| tb | 821.18 | K | Joback Method |
| tc | 1015.63 | K | Joback Method |
| tf | 493.61 | K | Joback Method |
| vc | 1.050 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 822.16 | J/mol×K | 821.18 | Joback Method |
| cpg | 836.09 | J/mol×K | 853.59 | Joback Method |
| cpg | 849.06 | J/mol×K | 886.00 | Joback Method |
| cpg | 861.10 | J/mol×K | 918.40 | Joback Method |
| cpg | 872.26 | J/mol×K | 950.81 | Joback Method |
| cpg | 882.58 | J/mol×K | 983.22 | Joback Method |
| cpg | 892.11 | J/mol×K | 1015.63 | Joback Method |

# Sources

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|---|---|
| **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=U346423&Units=SI |

# 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 |