# L-Valine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, hexyl ester

**Inchi:** InChI=1S/C19H25F4NO3/c1-4-5-6-7-11-27-18(26)16(12(2)3)24-17(25)13-9-8-10-14(15(1

**InchiKey:** NYKPIPRDDGFILM-UHFFFAOYSA-N

**Formula:** C19H25F4NO3

**SMILES:** CCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C

**Mol. weight [g/mol]:** 391.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -852.48 | kJ/mol | Joback Method |
| hf | -1329.56 | kJ/mol | Joback Method |
| hfus | 45.57 | kJ/mol | Joback Method |
| hvap | 78.49 | kJ/mol | Joback Method |
| log10ws | -6.17 | | Crippen Method |
| logp | 4.722 | | Crippen Method |
| mcvol | 280.880 | ml/mol | McGowan Method |
| pc | 1308.95 | kPa | Joback Method |
| rinpol | 2160.00 | | NIST Webbook |
| rinpol | 2160.00 | | NIST Webbook |
| tb | 844.06 | K | Joback Method |
| tc | 1039.97 | K | Joback Method |
| tf | 504.88 | K | Joback Method |
| vc | 1.105 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 879.77 | J/mol×K | 844.06 | Joback Method |
| cpg | 894.02 | J/mol×K | 876.71 | Joback Method |
| cpg | 907.27 | J/mol×K | 909.36 | Joback Method |
| cpg | 919.57 | J/mol×K | 942.01 | Joback Method |
| cpg | 930.96 | J/mol×K | 974.66 | Joback Method |
| cpg | 941.49 | J/mol×K | 1007.32 | Joback Method |
| cpg | 951.21 | J/mol×K | 1039.97 | Joback Method |

# Sources

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|---|---|
| **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=U346467&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |