# L-Valine, N-(2,6-difluorobenzoyl)-, hexyl ester

**Inchi:** InChI=1S/C18H25F2NO3/c1-4-5-6-7-11-24-18(23)16(12(2)3)21-17(22)15-13(19)9-8-10-1
**InchiKey:** PURSPZPABDNROW-UHFFFAOYSA-N
**Formula:** C18H25F2NO3
**SMILES:** CCCCCCOC(=O)C(NC(=O)c1c(F)cccc1F)C(C)C
**Mol. weight [g/mol]:** 341.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -474.12 | kJ/mol | Joback Method |
| hf | -907.95 | kJ/mol | Joback Method |
| hfus | 44.24 | kJ/mol | Joback Method |
| hvap | 79.19 | kJ/mol | Joback Method |
| log10ws | -5.40 | | Crippen Method |
| logp | 3.843 | | Crippen Method |
| mcvol | 263.250 | ml/mol | McGowan Method |
| pc | 1482.71 | kPa | Joback Method |
| rinpol | 2270.00 | | NIST Webbook |
| rinpol | 2270.00 | | NIST Webbook |
| tb | 825.87 | K | Joback Method |
| tc | 1023.86 | K | Joback Method |
| tf | 490.01 | K | Joback Method |
| vc | 1.024 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 805.88 | J/mol×K | 825.87 | Joback Method |
| cpg | 820.52 | J/mol×K | 858.87 | Joback Method |
| cpg | 834.14 | J/mol×K | 891.87 | Joback Method |
| cpg | 846.78 | J/mol×K | 924.86 | Joback Method |
| cpg | 858.45 | J/mol×K | 957.86 | Joback Method |
| cpg | 869.19 | J/mol×K | 990.86 | Joback Method |
| cpg | 879.03 | J/mol×K | 1023.86 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U346619&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |