# L-Valine, N-heptafluorobutyryl-, isobutyl ester

**Other names:** Val, isobutyl ester, HFB
Val, iso-Bu, HFB
**Inchi:** InChI=1S/C13H18F7NO3/c1-6(2)5-24-9(22)8(7(3)4)21-10(23)11(14,15)12(16,17)13(18,1
**InchiKey:** DVJZJVCXAFDQLN-UHFFFAOYSA-N
**Formula:** C13H18F7NO3
**SMILES:** CC(C)COC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
**Mol. weight [g/mol]:** 369.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -2207.06 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 27.66 | kJ/mol | Joback Method |
| hvap | 70.09 | kJ/mol | Cheméo Relay (1.0) |
| logp | 3.159 | | Crippen Method |
| mcvol | 225.410 | ml/mol | McGowan Method |
| pc | 1504.65 | kPa | Joback Method |
| tb | 484.18 | K | Cheméo Relay (1.0) |
| tc | 632.82 | K | Cheméo Relay (1.0) |
| tf | 312.02 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 662.59 | J/mol×K | 661.05 | Joback Method |
| cpg | 675.98 | J/mol×K | 688.98 | Joback Method |
| cpg | 688.53 | J/mol×K | 716.90 | Joback Method |
| cpg | 700.30 | J/mol×K | 744.83 | Joback Method |
| cpg | 711.33 | J/mol×K | 772.75 | Joback Method |
| cpg | 721.66 | J/mol×K | 800.68 | Joback Method |
| cpg | 731.33 | J/mol×K | 828.60 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U320895&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |

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