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

**Inchi:** InChI=1S/C14H20F7NO3/c1-4-5-6-7-25-10(23)9(8(2)3)22-11(24)12(15,16)13(17,18)14(1
**InchiKey:** RVLMKKYQGZADTK-UHFFFAOYSA-N
**Formula:** C14H20F7NO3
**SMILES:** CCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
**Mol. weight [g/mol]:** 383.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 33.77 | kJ/mol | Joback Method |
| log10ws | -5.12 | | Cheméo Relay (1.0) |
| logp | 3.693 | | Crippen Method |
| mcvol | 239.500 | ml/mol | McGowan Method |
| rinpol | 1423.00 | | NIST Webbook |
| rinpol | 1423.00 | | NIST Webbook |
| tb | 498.50 | K | Cheméo Relay (1.0) |
| tf | 306.98 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 715.56 | J/mol×K | 684.37 | Joback Method |
| cpg | 729.16 | J/mol×K | 712.12 | Joback Method |
| cpg | 741.94 | J/mol×K | 739.87 | Joback Method |
| cpg | 753.94 | J/mol×K | 767.61 | Joback Method |
| cpg | 765.22 | J/mol×K | 795.36 | Joback Method |
| cpg | 775.80 | J/mol×K | 823.11 | Joback Method |
| cpg | 785.74 | J/mol×K | 850.86 | Joback Method |

## Sources

**Cheméo Relay (1.0, beta):**

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U320897&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **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):** | |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |