# l-Valine, n-pentafluoropropionyl-, octadecyl ester

**Inchi:** InChI=1S/C26H46F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-35-23(33)22
**InchiKey:** IVCBSNVFTOZHSI-UHFFFAOYSA-N
**Formula:** C26H46F5NO3
**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
**Mol. weight [g/mol]:** 515.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1078.66 | kJ/mol | Joback Method |
| hf | -1892.49 | kJ/mol | Joback Method |
| hfus | 66.11 | kJ/mol | Joback Method |
| hvap | 88.35 | kJ/mol | Joback Method |
| log10ws | -9.38 | | Crippen Method |
| logp | 8.130 | | Crippen Method |
| mcvol | 405.040 | ml/mol | McGowan Method |
| pc | 706.21 | kPa | Joback Method |
| rinpol | 2620.00 | | NIST Webbook |
| tb | 963.62 | K | Joback Method |
| tc | 1195.91 | K | Joback Method |
| tf | 535.32 | K | Joback Method |
| vc | 1.613 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1413.61 | J/mol×K | 963.62 | Joback Method |
| cpg | 1434.72 | J/mol×K | 1002.34 | Joback Method |
| cpg | 1454.32 | J/mol×K | 1041.05 | Joback Method |
| cpg | 1472.57 | J/mol×K | 1079.77 | Joback Method |
| cpg | 1489.60 | J/mol×K | 1118.48 | Joback Method |
| cpg | 1505.56 | J/mol×K | 1157.20 | Joback Method |
| cpg | 1520.59 | J/mol×K | 1195.91 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U320892&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 |

# 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 |