# l-Leucine, n-pentafluoropropionyl-, nonyl ester

**Inchi:** InChI=1S/C18H30F5NO3/c1-4-5-6-7-8-9-10-11-27-15(25)14(12-13(2)3)24-16(26)17(19,2
**InchiKey:** CWRUPTFVKHMSIA-UHFFFAOYSA-N
**Formula:** C18H30F5NO3
**SMILES:** CCCCCCCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 403.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1146.02 | kJ/mol | Joback Method |
| hf | -1727.37 | kJ/mol | Joback Method |
| hfus | 45.39 | kJ/mol | Joback Method |
| hvap | 70.55 | kJ/mol | Joback Method |
| log10ws | -6.03 | | Crippen Method |
| logp | 5.009 | | Crippen Method |
| mcvol | 292.320 | ml/mol | McGowan Method |
| pc | 1114.82 | kPa | Joback Method |
| rinpol | 1814.00 | | NIST Webbook |
| tb | 780.58 | K | Joback Method |
| tc | 958.14 | K | Joback Method |
| tf | 445.16 | K | Joback Method |
| vc | 1.165 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 923.15 | J/mol×K | 780.58 | Joback Method |
| cpg | 939.02 | J/mol×K | 810.17 | Joback Method |
| cpg | 953.95 | J/mol×K | 839.77 | Joback Method |
| cpg | 968.01 | J/mol×K | 869.36 | Joback Method |
| cpg | 981.23 | J/mol×K | 898.95 | Joback Method |
| cpg | 993.67 | J/mol×K | 928.55 | Joback Method |
| cpg | 1005.37 | J/mol×K | 958.14 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321011&Units=SI |

# 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 |