# l-Isoleucine, n-pentafluoropropionyl-, decyl ester

**Inchi:** InChI=1S/C19H32F5NO3/c1-4-6-7-8-9-10-11-12-13-28-16(26)15(14(3)5-2)25-17(27)18(2

**InchiKey:** VOGQDFGPQBLICO-UHFFFAOYSA-N

**Formula:** C19H32F5NO3

**SMILES:** CCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)CC

**Mol. weight [g/mol]:** 417.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1137.60 | kJ/mol | Joback Method |
| hf | -1748.01 | kJ/mol | Joback Method |
| hfus | 47.98 | kJ/mol | Joback Method |
| hvap | 72.77 | kJ/mol | Joback Method |
| log10ws | -6.45 | | Crippen Method |
| logp | 5.399 | | Crippen Method |
| mcvol | 306.410 | ml/mol | McGowan Method |
| pc | 1046.65 | kPa | Joback Method |
| rinpol | 1929.00 | | NIST Webbook |
| tb | 803.46 | K | Joback Method |
| tc | 984.55 | K | Joback Method |
| tf | 456.43 | K | Joback Method |
| vc | 1.220 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 981.98 | J/mol×K | 803.46 | Joback Method |
| cpg | 998.31 | J/mol×K | 833.64 | Joback Method |
| cpg | 1013.67 | J/mol×K | 863.82 | Joback Method |
| cpg | 1028.12 | J/mol×K | 894.01 | Joback Method |
| cpg | 1041.70 | J/mol×K | 924.19 | Joback Method |
| cpg | 1054.47 | J/mol×K | 954.37 | Joback Method |
| cpg | 1066.48 | J/mol×K | 984.55 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U320871&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 |