# L-Phenylalanine, N-pentafluoropropionyl-, isohexyl ester

**Inchi:** InChI=1S/C18H22F5NO3/c1-12(2)7-6-10-27-15(25)14(11-13-8-4-3-5-9-13)24-16(26)17(1

**InchiKey:** JQUMOOLSHNOQGO-UHFFFAOYSA-N

**Formula:** C18H22F5NO3

**SMILES:** CC(C)CCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 395.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 39.43 | kJ/mol | Joback Method |
| log10ws | -5.22 | | Cheméo Relay (1.0) |
| logp | 3.891 | | Crippen Method |
| mcvol | 268.560 | ml/mol | McGowan Method |
| rinpol | 1839.00 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 832.97 | J/mol×K | 807.26 | Joback Method |
| cpg | 846.74 | J/mol×K | 839.45 | Joback Method |
| cpg | 859.54 | J/mol×K | 871.64 | Joback Method |
| cpg | 871.44 | J/mol×K | 903.84 | Joback Method |
| cpg | 882.49 | J/mol×K | 936.03 | Joback Method |
| cpg | 892.78 | J/mol×K | 968.22 | Joback Method |
| cpg | 902.35 | J/mol×K | 1000.41 | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U321021&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):**

**Cheméo Relay (1.0, beta):**

# 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 |