# l-Phenylalanine, n-pentafluoropropionyl-, heptadecyl ester

**Inchi:** InChI=1S/C29H44F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-38-26(36)25(23-2

**InchiKey:** DYEVCFBWRFGXBK-UHFFFAOYSA-N

**Formula:** C29H44F5NO3

**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 549.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -938.55 | kJ/mol | Joback Method |
| hf | -1712.60 | kJ/mol | Joback Method |
| hfus | 71.44 | kJ/mol | Joback Method |
| hvap | 97.70 | kJ/mol | Joback Method |
| log10ws | -9.98 | | Crippen Method |
| logp | 8.326 | | Crippen Method |
| mcvol | 423.550 | ml/mol | McGowan Method |
| pc | 719.53 | kPa | Joback Method |
| rinpol | 3055.00 | | NIST Webbook |
| rinpol | 3055.00 | | NIST Webbook |
| tb | 1059.38 | K | Joback Method |
| tc | 1318.63 | K | Joback Method |
| tf | 610.55 | K | Joback Method |
| vc | 1.679 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1498.99 | J/mol×K | 1059.38 | Joback Method |
| cpg | 1518.76 | J/mol×K | 1102.59 | Joback Method |
| cpg | 1537.16 | J/mol×K | 1145.80 | Joback Method |
| cpg | 1554.42 | J/mol×K | 1189.00 | Joback Method |
| cpg | 1570.77 | J/mol×K | 1232.21 | Joback Method |
| cpg | 1586.44 | J/mol×K | 1275.42 | Joback Method |
| cpg | 1601.66 | J/mol×K | 1318.63 | Joback Method |

# Sources

| | |
|---|---|
| **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=U321031&Units=SI |

# Legend

| | |
|---|---|
| **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 |