# D-Alanine, N-(2-fluoro-5-trifluoromethylbenzoyl)-, isohexyl ester

**Inchi:** InChI=1S/C17H21F4NO3/c1-10(2)5-4-8-25-16(24)11(3)22-15(23)13-9-12(17(19,20)21)6-
**InchiKey:** VWUPRGRHXMASQT-UHFFFAOYSA-N
**Formula:** C17H21F4NO3
**SMILES:** CC(C)CCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1F
**Mol. weight [g/mol]:** 363.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -869.32 | kJ/mol | Joback Method |
| hf | -1288.28 | kJ/mol | Joback Method |
| hfus | 40.39 | kJ/mol | Joback Method |
| hvap | 74.03 | kJ/mol | Joback Method |
| log10ws | -5.33 | | Crippen Method |
| logp | 3.942 | | Crippen Method |
| mcvol | 252.700 | ml/mol | McGowan Method |
| pc | 1511.67 | kPa | Joback Method |
| rinpol | 2008.00 | | NIST Webbook |
| rinpol | 2008.00 | | NIST Webbook |
| tb | 798.30 | K | Joback Method |
| tc | 991.98 | K | Joback Method |
| tf | 482.34 | K | Joback Method |
| vc | 0.994 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 765.41 | J/mol×K | 798.30 | Joback Method |
| cpg | 779.02 | J/mol×K | 830.58 | Joback Method |
| cpg | 791.69 | J/mol×K | 862.86 | Joback Method |
| cpg | 803.47 | J/mol×K | 895.14 | Joback Method |
| cpg | 814.39 | J/mol×K | 927.42 | Joback Method |
| cpg | 824.50 | J/mol×K | 959.70 | Joback Method |
| cpg | 833.82 | J/mol×K | 991.98 | Joback Method |

# Sources

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|---|---|
| **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=U348347&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |