# D-Alanine, N-(3-fluoro-5-trifluoromethylbenzoyl)-, octadecyl ester

**Inchi:** InChI=1S/C29H45F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-37-28(36)23(
**InchiKey:** AJPOZBPJMIXUHF-UHFFFAOYSA-N
**Formula:** C29H45F4NO3
**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)cc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 531.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -765.84 | kJ/mol | Joback Method |
| hf | -1530.68 | kJ/mol | Joback Method |
| hfus | 75.00 | kJ/mol | Joback Method |
| hvap | 101.13 | kJ/mol | Joback Method |
| log10ws | -10.60 | | Crippen Method |
| logp | 8.768 | | Crippen Method |
| mcvol | 421.780 | ml/mol | McGowan Method |
| pc | 717.99 | kPa | Joback Method |
| rinpol | 3112.00 | | NIST Webbook |
| tb | 1073.30 | K | Joback Method |
| tc | 1339.36 | K | Joback Method |
| tf | 632.58 | K | Joback Method |
| vc | 1.671 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1490.98 | J/mol×K | 1073.30 | Joback Method |
| cpg | 1510.37 | J/mol×K | 1117.64 | Joback Method |
| cpg | 1528.00 | J/mol×K | 1161.99 | Joback Method |
| cpg | 1544.05 | J/mol×K | 1206.33 | Joback Method |
| cpg | 1558.69 | J/mol×K | 1250.67 | Joback Method |
| cpg | 1572.10 | J/mol×K | 1295.01 | Joback Method |
| cpg | 1584.47 | J/mol×K | 1339.36 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U347817&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 |

# 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 |

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