# L-Valine, N-(3-fluorobenzoyl)-, pentadecyl ester

**Inchi:** InChI=1S/C27H44FNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-32-27(31)25(22(2)3)29
**InchiKey:** HAAIWEURSDXUEP-UHFFFAOYSA-N
**Formula:** C27H44FNO3
**SMILES:** CCCCCCCCCCCCCCCOC(=O)C(N=C(O)c1cccc(F)c1)C(C)C
**Mol. weight [g/mol]:** 449.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -906.82 | kJ/mol | Joback Method |
| hvap | 106.27 | kJ/mol | Joback Method |
| log10ws | -8.38 | | Crippen Method |
| logp | 7.789 | | Crippen Method |
| mcvol | 388.290 | ml/mol | McGowan Method |
| pc | 823.37 | kPa | Joback Method |
| rinpol | 3146.00 | | NIST Webbook |
| rinpol | 3146.00 | | NIST Webbook |
| tb | 1092.24 | K | Joback Method |
| tc | 1352.40 | K | Joback Method |

## Sources

**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=U346681&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

**hf:** Enthalpy of formation 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 |