

L-Valine, N-(4-fluoro-2-trifluoromethylbenzoyl)-, propyl

Inchi:
ester

InChI=1S/C16H19F4NO3/c1-4-7-24-15(23)13(9(2)3)21-14(22)11-6-5-10(17)8-12(11)16(1

InchiKey:

FCYIDLULVXISIL-UHFFFAOYSA-N

Formula:

C16H19F4NO3

SMILES:

CCCOC(=O)C(NC(=O)c1ccc(F)cc1C(F)(F)F)C(C)C

Mol. weight [g/mol]:

349.32

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -877.74 | kJ/mol | Joback Method |
| hf | -1267.64 | kJ/mol | Joback Method |
| hfus | 37.80 | kJ/mol | Joback Method |
| hvap | 71.81 | kJ/mol | Joback Method |
| log10ws | -4.91 | | Crippen Method |
| logp | 3.552 | | Crippen Method |
| mcvol | 238.610 | ml/mol | McGowan Method |
| pc | 1631.17 | kPa | Joback Method |
| rinpol | 1874.00 | | NIST Webbook |
| rinpol | 1874.00 | | NIST Webbook |
| tb | 775.42 | K | Joback Method |
| tc | 968.98 | K | Joback Method |
| tf | 471.07 | K | Joback Method |
| vc | 0.938 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 709.57 | J/mol×K | 775.42 | Joback Method |
| cpg | 722.86 | J/mol×K | 807.68 | Joback Method |
| cpg | 735.23 | J/mol×K | 839.94 | Joback Method |
| cpg | 746.73 | J/mol×K | 872.20 | Joback Method |
| cpg | 757.39 | J/mol×K | 904.46 | Joback Method |
| cpg | 767.26 | J/mol×K | 936.72 | Joback Method |
| cpg | 776.36 | J/mol×K | 968.98 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U346479&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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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