# «beta»-alanine, trifluoroacetyl-isopropyl ester

**Inchi:** InChI=1S/C8H12F3NO3/c1-5(2)15-6(13)3-4-12-7(14)8(9,10)11/h5H,3-4H2,1-2H3,(H,12,1
**InchiKey:** JPHKRJVNMJIUJE-UHFFFAOYSA-N
**Formula:** C8H12F3NO3
**SMILES:** CC(C)OC(=O)CCNC(=O)C(F)(F)F
**Mol. weight [g/mol]:** 227.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -841.00 | kJ/mol | Joback Method |
| hf | -1114.72 | kJ/mol | Joback Method |
| hfus | 24.26 | kJ/mol | Joback Method |
| hvap | 51.60 | kJ/mol | Joback Method |
| log10ws | -1.77 | | Crippen Method |
| logp | 1.007 | | Crippen Method |
| mcvol | 147.880 | ml/mol | McGowan Method |
| pc | 2571.50 | kPa | Joback Method |
| rinpol | 1160.00 | | NIST Webbook |
| tb | 556.91 | K | Joback Method |
| tc | 732.53 | K | Joback Method |
| tf | 343.86 | K | Joback Method |
| vc | 0.586 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 374.04 | J/mol×K | 556.91 | Joback Method |
| cpg | 385.25 | J/mol×K | 586.18 | Joback Method |
| cpg | 395.88 | J/mol×K | 615.45 | Joback Method |
| cpg | 405.93 | J/mol×K | 644.72 | Joback Method |
| cpg | 415.43 | J/mol×K | 673.99 | Joback Method |
| cpg | 424.40 | J/mol×K | 703.26 | Joback Method |
| cpg | 432.84 | J/mol×K | 732.53 | 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=R267799&Units=SI |

# 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 |