

2-Amino-2-methylpropan-1-ol, N-pentafluoropropionyl

Other names: 2,2,3,3,3-Pentafluoro-N-(1-hydroxy-2-methylpropan-2-yl)propanamide
Inchi: InChI=1S/C7H10F5NO2/c1-5(2,3-14)13-4(15)6(8,9)7(10,11)12/h14H,3H2,1-2H3,(H,13,15)
InchiKey: SRZZIOLRYMDSIP-UHFFFAOYSA-N
Formula: C7H10F5NO2
SMILES: CC(C)(CO)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 235.15

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| gf | -1133.82 | kJ/mol | Joback Method |
| hf | -1405.95 | kJ/mol | Joback Method |
| hfus | 17.83 | kJ/mol | Joback Method |
| hvap | 53.06 | kJ/mol | Joback Method |
| log10ws | -2.07 | | Crippen Method |
| logp | 1.071 | | Crippen Method |
| mcvol | 135.760 | ml/mol | McGowan Method |
| pc | 2799.47 | kPa | Joback Method |
| rinpol | 991.00 | | NIST Webbook |
| rinpol | 991.00 | | NIST Webbook |
| tb | 542.44 | K | Joback Method |
| tc | 705.20 | K | Joback Method |
| tf | 342.27 | K | Joback Method |
| vc | 0.544 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 362.75 | J/molxK | 542.44 | Joback Method |
| cpg | 372.58 | J/molxK | 569.57 | Joback Method |
| cpg | 381.75 | J/molxK | 596.69 | Joback Method |
| cpg | 390.28 | J/molxK | 623.82 | Joback Method |
| cpg | 398.21 | J/molxK | 650.95 | Joback Method |
| cpg | 405.60 | J/molxK | 678.08 | Joback Method |
| cpg | 412.47 | J/molxK | 705.20 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U378713&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 |
| 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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