

6-Amino-1-hexanol, N,O-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C12H13F10NO3/c13-9(14,11(17,18)19)7(24)23-5-3-1-2-4-6-26-8(25)10(15,16)
InchiKey: MVMRMDCCFHBSKH-UHFFFAOYSA-N
Formula: C12H13F10NO3
SMILES: O=C(NCCCCCOC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 409.22

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| gf | -2160.03 | kJ/mol | Joback Method |
| hf | -2591.02 | kJ/mol | Joback Method |
| hfus | 37.46 | kJ/mol | Joback Method |
| hvap | 51.29 | kJ/mol | Joback Method |
| log10ws | -4.63 | | Crippen Method |
| logp | 3.601 | | Crippen Method |
| mcvol | 216.630 | ml/mol | McGowan Method |
| pc | 1454.57 | kPa | Joback Method |
| rinpol | 1357.00 | | NIST Webbook |
| tb | 634.07 | K | Joback Method |
| tc | 787.74 | K | Joback Method |
| tf | 415.33 | K | Joback Method |
| vc | 0.908 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 636.13 | J/molxK | 634.07 | Joback Method |
| cpg | 647.77 | J/molxK | 659.68 | Joback Method |
| cpg | 658.67 | J/molxK | 685.29 | Joback Method |
| cpg | 668.87 | J/molxK | 710.90 | Joback Method |
| cpg | 678.41 | J/molxK | 736.52 | Joback Method |
| cpg | 687.34 | J/molxK | 762.13 | Joback Method |
| cpg | 695.70 | J/molxK | 787.74 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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=U375564&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 |
| 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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