

Heptafluorobutanamide, N,N-bis(2-ethylhexyl)-

Inchi: InChI=1S/C20H34F7NO/c1-5-9-11-15(7-3)13-28(14-16(8-4)12-10-6-2)17(29)18(21,22)19
InchiKey: DRDRAZUGOVAKNM-UHFFFAOYSA-N
Formula: C20H34F7NO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 437.48

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -1260.65 | kJ/mol | Joback Method |
| hf | -1910.76 | kJ/mol | Joback Method |
| hfus | 44.45 | kJ/mol | Joback Method |
| hvap | 58.52 | kJ/mol | Joback Method |
| log10ws | -7.35 | | Crippen Method |
| logp | 7.081 | | Crippen Method |
| mcvol | 316.600 | ml/mol | McGowan Method |
| pc | 907.79 | kPa | Joback Method |
| rinpol | 1724.00 | | NIST Webbook |
| tb | 707.63 | K | Joback Method |
| tc | 869.17 | K | Joback Method |
| tf | 378.95 | K | Joback Method |
| vc | 1.260 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 977.90 | J/mol×K | 707.63 | Joback Method |
| cpg | 996.14 | J/mol×K | 734.55 | Joback Method |
| cpg | 1013.40 | J/mol×K | 761.48 | Joback Method |
| cpg | 1029.75 | J/mol×K | 788.40 | Joback Method |
| cpg | 1045.24 | J/mol×K | 815.32 | Joback Method |
| cpg | 1059.94 | J/mol×K | 842.25 | Joback Method |
| cpg | 1073.89 | J/mol×K | 869.17 | 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=U308273&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 |
| mccvol: | 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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