

N-benzyl-1,1,1-trifluoromethanesulphonamide

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|-----------------------------|---|
| Inchi: | InChI=1S/C8H8F3NO2S/c9-8(10,11)15(13,14)12-6-7-4-2-1-3-5-7/h1-5,12H,6H2 |
| InchiKey: | IJHVVEQTOXFGCL-UHFFFAOYSA-N |
| Formula: | C8H8F3NO2S |
| SMILES: | O=S(=O)(NCc1ccccc1)C(F)(F)F |
| Mol. weight [g/mol]: | 239.22 |
| CAS: | 36457-58-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -831.85 | kJ/mol | Joback Method |
| hf | -968.88 | kJ/mol | Joback Method |
| hfus | 28.82 | kJ/mol | Joback Method |
| hvap | 57.00 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 1.626 | | Crippen Method |
| mcvol | 143.200 | ml/mol | McGowan Method |
| pc | 3891.64 | kPa | Joback Method |
| tb | 501.65 | K | Joback Method |
| tc | 689.25 | K | Joback Method |
| tf | 301.75 | K | Joback Method |
| vc | 0.580 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 322.71 | J/molxK | 501.65 | Joback Method |
| cpg | 335.34 | J/molxK | 532.92 | Joback Method |
| cpg | 347.15 | J/molxK | 564.18 | Joback Method |
| cpg | 358.18 | J/molxK | 595.45 | Joback Method |
| cpg | 368.46 | J/molxK | 626.71 | Joback Method |
| cpg | 378.01 | J/molxK | 657.98 | Joback Method |
| cpg | 386.85 | J/molxK | 689.25 | 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=C36457586&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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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