

benzene-1,4-disulfonamide

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| Inchi: | InChI=1S/C6H8N2O4S2/c7-13(9,10)5-1-2-6(4-3-5)14(8,11)12/h1-4H,(H2,7,9,10)(H2,8,11) |
| InchiKey: | WOUBWJAJSXAOIV-UHFFFAOYSA-N |
| Formula: | C6H8N2O4S2 |
| SMILES: | NS(=O)(=O)c1ccc(S(N)(=O)=O)cc1 |
| Mol. weight [g/mol]: | 236.27 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|--------------------------------------|
| gf | -701.76 | kJ/mol | Joback Method |
| hf | -781.23 | kJ/mol | Joback Method |
| hfus | 38.10 | kJ/mol | Joback Method |
| hvap | 90.44 | kJ/mol | Joback Method |
| log10ws | -2.53 | | Aqueous Solubility Prediction Method |
| logp | -1.019 | | Crippen Method |
| mcvol | 147.780 | ml/mol | McGowan Method |
| pc | 9001.58 | kPa | Joback Method |
| tb | 608.96 | K | Joback Method |
| tc | 832.10 | K | Joback Method |
| tf | 439.96 | K | Joback Method |
| vc | 0.574 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 346.43 | J/molxK | 608.96 | Joback Method |
| cpg | 357.43 | J/molxK | 646.15 | Joback Method |
| cpg | 367.58 | J/molxK | 683.34 | Joback Method |
| cpg | 376.86 | J/molxK | 720.53 | Joback Method |
| cpg | 385.28 | J/molxK | 757.72 | Joback Method |
| cpg | 392.80 | J/molxK | 794.91 | Joback Method |
| cpg | 399.42 | J/molxK | 832.10 | Joback Method |

Sources

| | |
|--|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| Aqueous Solubility Prediction Method: | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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