

8-Hydroxyquinoline-5-sulfonic acid

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| Other names: | 5-Quinolinesulfonic acid, 8-hydroxy-Oxine-5-sulfonic acid 5-Sulfo-8-hydroxyquinoline 5-Sulfo-8-quinolinol 5-Sulfooxine 8-Hydroxy-5-quinolinesulfonic acid 8-Hydroxy-5-sulfoquinoline 8-Hydroxyquinoline-5-sulfonate 8-Hydroxyquinoline-5-sulphonic acid 8-Quinolinol-5-sulfonic acid Sulfoxine 8-Oxyquinoline-5-sulfonic acid NSC 13139 |
| Inchi: | InChI=1S/C9H7NO4S/c11-7-3-4-8(15(12,13)14)6-2-1-5-10-9(6)7/h1-5,11H,(H,12,13,14) |
| InchiKey: | LGDFHDKSYGVKDC-UHFFFAOYSA-N |
| Formula: | C9H7NO4S |
| SMILES: | O=S(=O)(O)c1ccc(O)c2ncccc12 |
| Mol. weight [g/mol]: | 225.22 |
| CAS: | 84-88-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.18 | | Crippen Method |
| logp | 1.187 | | Crippen Method |
| mcpvol | 144.260 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C84888&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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