

4-Hydroxybenzo[b]thiophene

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|-----------------------------|--|
| Other names: | Benzo[b]thiophene-4-ol 4-Hydroxybenzothiophene 1-Benzothiophene-4-ol |
| Inchi: | InChI=1S/C8H6OS/c9-7-2-1-3-8-6(7)4-5-10-8/h1-5,9H |
| InchiKey: | BMRZGYNNZTVECK-UHFFFAOYSA-N |
| Formula: | C8H6OS |
| SMILES: | Oc1cccc2sccc12 |
| Mol. weight [g/mol]: | 150.20 |
| CAS: | 3610-02-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.58 | | Crippen Method |
| logp | 2.607 | | Crippen Method |
| mcvol | 106.880 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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=C3610024&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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