

1H-Benzimidazole, 2-(methylthio)-

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|-----------------------------|---|
| Other names: | Benzimidazole, 2-(methylthio)- S-Methyl-2-mercaptobenzimidazole 2-(Methylmercapto)benzimidazole 2-(Methylthio)benzimidazole 2-Methylsulfanyl-1H-benzimidazole 2-(Methylsulfanyl)-1H-benzimidazole NSC 21699 |
| Inchi: | InChI=1S/C8H8N2S/c1-11-8-9-6-4-2-3-5-7(6)10-8/h2-5H,1H3,(H,9,10) |
| InchiKey: | OCKJFOHZLXIAAT-UHFFFAOYSA-N |
| Formula: | C8H8N2S |
| SMILES: | CSc1nc2ccccc2[nH]1 |
| Mol. weight [g/mol]: | 164.23 |
| CAS: | 7152-24-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.00 | | Crippen Method |
| logp | 1.803 | | Crippen Method |
| mvol | 120.970 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C7152241&Units=SI |
| 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 |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |

mcvol: McGowan's characteristic volume

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