

6-Methyl, 2-methylmercapto-4-oxo-1,3,3a,7-tetrazaindene

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|----------------------|--|
| Inchi: | InChI=1S/C7H8N4OS/c1-4-3-5(12)11-6(8-4)9-7(10-11)13-2/h3H,1-2H3,(H,8,9,10) |
| InchiKey: | DITIBSDLGMCMTU-UHFFFAOYSA-N |
| Formula: | C7H8N4OS |
| SMILES: | CSc1nc2[nH]c(C)cc(=O)n2n1 |
| Mol. weight [g/mol]: | 196.23 |
| CAS: | 89853-03-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.82 | | Crippen Method |
| logp | -0.034 | | Crippen Method |
| mcvol | 132.710 | ml/mol | McGowan Method |

Sources

| | |
|-----------------|---|
| 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=C89853032&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/11-040-4/6-Methyl-2-methylmercapto-4-oxo-1-3-3a-7-tetrazaindene.pdf>

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