

1H-Tetrazole-5-thiol, 1-phenyl-

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|-----------------------------|---|
| Other names: | Mercaptophenyltetrazole Phenylmercaptotetrazole 1-Phenyl-5-mercaptotetrazole 1-Phenyl-5-tetrazolethione 1-Phenyltetrazole-5-thiol 1-Phenyltetrazolethiol 5-Mercapto-1-phenyltetrazol 5-Mercapto-1-phenyltetrazole 1-Phenyl-1H-tetrazole-5-thiol 5-Mercapto-1-phenyl-1,2,3,4-tetrazole 1-Phenyl-5-mercapto-1,2,3,4-tetrazole 1-Phenyl-5-mercapto-1H-tetrazole 1,2,3,4-Tetrazole-5-thiol, 1-phenyl- 1-Phenyltetrazoline-5-thione 2-Tetrazoline-5-thione, 1-phenyl- 5H-Tetrazole-5-thione, 1,2-dihydro-1-phenyl- NSC 24018 |
| Inchi: | InChI=1S/C7H6N4S/c12-7-8-9-10-11(7)6-4-2-1-3-5-6/h1-5H,(H,8,10,12) |
| InchiKey: | GGZHVNZHFYCSEV-UHFFFAOYSA-N |
| Formula: | C7H6N4S |
| SMILES: | Sc1nnnn1-c1ccccc1 |
| Mol. weight [g/mol]: | 178.21 |
| CAS: | 86-93-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.93 | | Crippen Method |
| logp | 0.951 | | Crippen Method |
| mcvol | 122.540 | 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=C86931&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

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