

2H-Imidazole-2-thione, 1,3-dihydro-1-methyl-

Other names:

- 1,3-Dihydro-1-methyl-2H-imidazole-2-thione
- 1-Methyl-1,3-dihydroimidazole-2-thione
- 1-Methyl-2-imidazolethiol
- 1-Methylimidazole-2(3H)-thione
- 1-Methylimidazole-2-thione
- 1-Metylo 2 merkaptimidazole
- 1-methyl-2-mercaptimidazole
- 1-methylimidazole-2-thiol
- 2-Mercapto-1-methylimidazole
- 4-Imidazoline-2-thione, 1-methyl-
- Basolan
- Danantizol
- Favistan
- Frentirox
- Imidazole, 1-methyl-2-mercapto-
- Imidazole-2-thio, 1-methyl-
- Mercasolyl
- Mercazolyl
- Merkastan
- Merkazolil
- Methiamazole
- Methimazol
- Metizol
- Metothylin
- Metothyline
- Metotirin
- N-Methyl-2-mercaptimidazole
- Strumazol
- Strumazole
- Tapazole
- Tapuzole
- Thacapzol
- Thiamazol
- Thiamazole
- Thimazole
- Thycapsol
- Thycapzol
- Thymidazol
- Thymidazole
- USAF EL-30

imidazole-2-thiol, 1-methyl-
 mercaptazole
 mercazole
 metazolo
 methimazole
 methylmercaptoimidazole
Inchi: InChI=1S/C4H6N2S/c1-6-3-2-5-4(6)7/h2-3H,1H3,(H,5,7)
InchiKey: PMRYVIKBURPHAH-UHFFFAOYSA-N
Formula: C4H6N2S
SMILES: Cn1ccnc1S
Mol. weight [g/mol]: 114.17
CAS: 60-56-0

Physical Properties

Property code	Value	Unit	Source
ie	7.41 ± 0.03	eV	NIST Webbook
log10ws	-3.04		Crippen Method
logp	0.709		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
tf	418.60	K	Thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of three sulfur imidazole derivatives

Sources

Thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of three sulfur imidazole derivatives: Methimazole, Methymercaptazole, and Iodoquinoline in Supercritical Carbon Dioxide:
 NIST Webbook:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1016/j.jct.2018.03.002>

<https://www.doi.org/10.1021/je020080h>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C60560&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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