

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 merkaptoimidazolem
1-methyl-2-mercaptoimidazole
1-methylimidazole-2-thiol
2-Mercapto-1-methylimidazole
4-Imidazoline-2-thione, 1-methyl-
Basolan
Danantizol
Favistan
Frentirox
Imidazole, 1-methyl-2-mercaptop-
Imidazole-2-thio, 1-methyl-
Mercasolyl
Mercazolyl
Merkastan
Merkazolil
Methiamazole
Methimazol
Metizol
Metothyryin
Metothyryne
Metotirin
N-Methyl-2-mercaptopimidazole
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60560&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of three sulfur imidazole derivatives	https://www.doi.org/10.1016/j.jct.2018.03.002
Relationships between Physicochemical Properties of Methylparaben, and Methylparaben in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je020080h http://link.springer.com/article/10.1007/BF02311772

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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