

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

Other names:	Imidazole-2-thiol 1,3-Vinylenethiourea 1H-Imidazole-2-thiol 2-Mercaptoimidazole 2-Thioxo-2,3-dihydroimidazole 4-Imidazoline-2-thione Imidazole, 2-mercapto- USAF EL-57 1,3-Dihydro-2H-imidazole-2-thione 2-Mercapto-1H-imidazole NSC 112715
Inchi:	InChI=1S/C3H4N2S/c6-3-4-1-2-5-3/h1-2H,(H2,4,5,6)
InchiKey:	OXFSTTJBVAAALW-UHFFFAOYSA-N
Formula:	C3H4N2S
SMILES:	<chem>Sc1ncc[nH]1</chem>
Mol. weight [g/mol]:	100.14
CAS:	872-35-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	0.217		Crippen Method
mcvol	69.980	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C872355&Units=SI

Legend

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

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