

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

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
mccvol	122.540	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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>

Legend

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

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