

2-Amino-5-mercapto-1,3,4-thiadiazole

Other names:	2-Amino-5-mercapto-1,3,4-thiadiazole
	5-Amino-2-mercapto-1,3,4-thiadiazole
	2-Amino-1,3,4-thiadiazole-5-mercaptan
	2-Amino-1,3,4-thiadiazole-5-thiol
	5-Amino-1,3,4-thiadiazole-2-thiol
	2-Amino-«delta»2-1,3,4-thiadiazoline-5-thione
	5-Amino-1,3,4-thiadiazoline-2-thione
	2-Mercapto-5-amino-1,3,4-thiadiazole
	1,3,4-Thiadiazole-2-thiol, 5-amino-
	«DELTA»2-1,3,4-Thiadiazoline-2-thiol, 5-imino-
	2-Thiol-5-amino-1,3,4-thiadiazole
	2-Amino-5-mercaptothiadiazole
	USAF PD-25
	NSC 21402
	5-Amino-1,3,4-thiadiazole-2(3H)-thione
	5-Thiol-2-amino-1,3,4-thiadiazole
Inchi:	InChI=1S/C2H3N3S2/c3-1-4-5-2(6)7-1/h(H2,3,4)(H,5,6)
InchiKey:	GDGIVSREGUOIJZ-UHFFFAOYSA-N
Formula:	C2H3N3S2
SMILES:	Nc1nnc(S)s1
Mol. weight [g/mol]:	133.20

Physical Properties

Property code	Value	Unit	Source
ie	8.21	eV	Cheméo Relay (1.0)
logp	0.409		Crippen Method
mcvol	82.220	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
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2349679&Units=SI>

McGowan Method:

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

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/32-344-4/2-Amino-5-mercapto-1-3-4-thiadiazole.pdf>

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