

1,3,4-Thiadiazol-2-amine

Other names:	Aminothiadiazole
	2-Aminothiadiazole
	2-Amino-1,3,4-thiadiazole
	NSC 4728
	TF 128
	1,3,4-Thiadiazole-2-amine
	1,3,4-Thiadiazole, 2-amino-
	ATDA
	FDA 0084
	X 26
	2-Amino-1-thia-3,4-diazole
	[1,3,4]Thiadiazol-2-ylamine
Inchi:	InChI=1S/C2H3N3S/c3-2-5-4-1-6-2/h1H,(H2,3,5)
InchiKey:	QUKGLNCXGVWCJX-UHFFFAOYSA-N
Formula:	C2H3N3S
SMILES:	Nc1nncs1
Mol. weight [g/mol]:	101.13

Physical Properties

Property code	Value	Unit	Source
logp	0.120		Crippen Method
mcvol	65.870	ml/mol	McGowan Method

Sources

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=C4005510&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/67-239-3/1-3-4-Thiadizol-2-amine.pdf>

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