

1,2,4-Thiadiazole, 5-amino-

Other names:	1,2,4-Thiadiazol-5-amine 5-Amino-1,2,4-thiadiazole
Inchi:	InChI=1S/C2H3N3S/c3-2-4-1-5-6-2/h1H,(H2,3,4,5)
InchiKey:	VJHTZTZOKVQRN-UHFFFAOYSA-N
Formula:	C2H3N3S
SMILES:	<chem>N=c1nc[nH]s1</chem>
Mol. weight [g/mol]:	101.13
CAS:	7552-07-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.21		Crippen Method
logp	-0.531		Crippen Method
mcvol	65.870	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7552070&Units=SI
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

Legend

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

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