

# Thiadiazolo[3,4-d]pyrimidine-5-thiol, 1,2,5-, 7-amino-

Inchi:	InChI=1S/C4H3N5S2/c5-2-1-3(9-11-8-1)7-4(10)6-2/h(H3,5,6,7,9,10)
InchiKey:	FDSKBIARWAZXIA-UHFFFAOYSA-N
Formula:	C4H3N5S2
SMILES:	N=c1nc(S)nc2[nH]snc1-2
Mol. weight [g/mol]:	185.23
CAS:	90773-36-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	-0.348		Crippen Method
mcvol	110.900	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C90773367&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90773367&amp;Units=SI</a>

## Legend

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

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