

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
CAS:	4005-51-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.39		Crippen Method
logp	0.120		Crippen Method
mcvol	65.870	ml/mol	McGowan Method

Sources

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=C4005510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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