

2-Nitramino-1,3,4-thiadiazole

Inchi:	InChI=1S/C2H2N4O2S/c7-6(8)5-2-4-3-1-9-2/h1H,(H,4,5)
InchiKey:	CCPANCYSEDJEPB-UHFFFAOYSA-N
Formula:	C2H2N4O2S
SMILES:	O=[N+](O-)[Nc1nncs1
Mol. weight [g/mol]:	146.13
CAS:	26947-66-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	0.142		Crippen Method
mcvol	83.290	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26947660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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