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/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