

1,2,5-Thiadiazole-3-carboxamidoxime, 4-(hydroxyiminomethylamino)-

Inchi: InChI=1S/C4H6N6O2S/c5-3(8-12)2-4(6-1-7-11)10-13-9-2/h1,11-12H,(H2,5,8)(H,6,7,10)
InchiKey: LOKUKLGCLSCCKLO-UHFFFAOYSA-N
Formula: C4H6N6O2S
SMILES: N=C(NO)c1nsnc1NC=NO
Mol. weight [g/mol]: 202.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	-0.328		Crippen Method
mcvol	127.130	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=B6008434&Units=SI>

Legend

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

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