

3-Thiomorpholinemethanol, s-hydrogenthiosulfate

Inchi:	InChI=1S/C5H11NO3S3/c7-12(8,9)11-4-5-3-10-2-1-6-5/h5-6H,1-4H2,(H,7,8,9)
InchiKey:	YVJPWJQJQLRLPT-UHFFFAOYSA-N
Formula:	C5H11NO3S3
SMILES:	O=S(=O)([O-])SCC1CSCC[NH2+]1
Mol. weight [g/mol]:	229.34

Physical Properties

Property code	Value	Unit	Source
log10ws	0.97		Crippen Method
logp	-1.141		Crippen Method
mcvol	147.090	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=B6006861&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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