

Octylthiosulfuric acid, 2-amino-2-methyl-

Inchi:	InChI=1S/C9H21NO3S2/c1-3-4-5-6-7-9(2,10)8-14-15(11,12)13/h3-8,10H2,1-2H3,(H,11,1
InchiKey:	OJYNSCSZMGARGK-UHFFFAOYSA-N
Formula:	C9H21NO3S2
SMILES:	CCCCCCC(C)([NH3+])CSS(=O)(=O)[O-]
Mol. weight [g/mol]:	255.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.51		Crippen Method
logp	1.151		Crippen Method
mcvol	197.960	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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