

Ethylthiosulfuric acid, 2-[(1,7,7-trimethylbicyclo[2.2.1.]hept-2-yl)-amino]-

Inchi: InChI=1S/C12H23NO3S2/c1-11(2)9-4-5-12(11,3)10(8-9)13-6-7-17-18(14,15)16/h9-10,13
InchiKey: WYGZEEQGKUVVVGU-UHFFFAOYSA-N
Formula: C12H23NO3S2
SMILES: CC1(C)C2CCC1(C)C([NH2+])CCSS(=O)(=O)[O-]C2
Mol. weight [g/mol]: 293.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	0.958		Crippen Method
mcvol	218.510	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=B6010459&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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