

# Thiosulfuric acid, s-[2-[(2-anilinoethyl)amino]ethyl]ester

Inchi:	InChI=1S/C10H16N2O3S2/c13-17(14,15)16-9-8-11-6-7-12-10-4-2-1-3-5-10/h1-5,11-12H
InchiKey:	MKLXZHHTNGKIQR-UHFFFAOYSA-N
Formula:	C10H16N2O3S2
SMILES:	O=S(=O)([O-])SCC[NH2+]CCNc1ccccc1
Mol. weight [g/mol]:	276.38
CAS:	23563-74-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.04		Crippen Method
logp	-0.145		Crippen Method
mvol	198.270	ml/mol	McGowan Method

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23563748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23563748&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/115-752-9/Thiosulfuric-acid-s-2-2-anilinoethyl-amino-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-29 11:46:25.325141433 +0000 UTC m=+16680434.245718745.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.