

Rhodanine, 3-salicylideneamino-

Inchi:	InChI=1S/C10H8N2O2S2/c13-8-4-2-1-3-7(8)5-11-12-9(14)6-16-10(12)15/h1-5,13H,6H2/
InchiKey:	MFYPPBDQQGTAFD-VZUCSPMQSA-N
Formula:	C10H8N2O2S2
SMILES:	O=C1CSC(=S)N1N=Cc1ccccc1O
Mol. weight [g/mol]:	252.31
CAS:	35533-29-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.586		Crippen Method
mcvol	168.640	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=C35533290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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<https://www.chemeo.com/cid/61-525-1/Rhodanine-3-salicylideneamino.pdf>

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