

Rhodanine, 3-amino-5-benzylidene-

Inchi:	InChI=1S/C10H8N2OS2/c11-12-9(13)8(15-10(12)14)6-7-4-2-1-3-5-7/h1-6H,11H2/b8-6+
InchiKey:	RADJDINPADSTBJ-SOFGYWHQSA-N
Formula:	C10H8N2OS2
SMILES:	NN1C(=O)C(=Cc2ccccc2)SC1=S
Mol. weight [g/mol]:	236.31
CAS:	4992-29-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	1.762		Crippen Method
mcvol	162.770	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=C4992294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/54-988-6/Rhodanine-3-amino-5-benzylidene.pdf>

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