

Rhodanine, 5-(2-furfurylidene)-

Inchi:	InChI=1S/C8H5NO2S2/c10-7-6(13-8(12)9-7)4-5-2-1-3-11-5/h1-4H,(H,9,10,12)/b6-4+
InchiKey:	ISSUVJNRFWFRIV-GQCTYLIASA-N
Formula:	C8H5NO2S2
SMILES:	O=C1NC(=S)SC1=Cc1cccO1
Mol. weight [g/mol]:	211.26
CAS:	4703-96-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	1.768		Crippen Method
mcvol	134.780	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4703962&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/44-246-0/Rhodanine-5-2-furfurylidene.pdf>

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