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/b
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