2-Mercaptothiazole

Other names: 2-Thiazolethiol
Inchi: InChI=1S/C3H3NS2/c5-3-4-1-2-6-3/h1-2H,(H,4,5)
InchiKey: OCVLSHAVSIYKLI-UHFFFAOYSA-N
Formula: C3H3NS2
SMILES: Sc1nccs1
Mol. weight [g/mol]: 117.19
CAS: 82358-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	1.432		Crippen Method
mcvol	76.350	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C82358096&Units=SI

Legend

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