

5-Chloro-2-thienyl methyl ketone thiosemicarbazone

Inchi:	InChI=1S/C7H8ClN3S2/c1-4(10-11-7(9)12)5-2-3-6(8)13-5/h2-3H,1H3,(H3,9,11,12)/b10-4
InchiKey:	APCFEGJUKJTYCB-WMZJFQQLSA-N
Formula:	C7H8ClN3S2
SMILES:	CC(=NNC(N)=S)c1ccc(Cl)s1
Mol. weight [g/mol]:	233.74
CAS:	79155-44-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	1.959		Crippen Method
mcvol	156.310	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79155445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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