

Semicarbazide, 1-(5-nitro-2-furoyl)-3-thio-

Inchi:	InChI=1S/C6H6N4O4S/c7-6(15)9-8-5(11)3-1-2-4(14-3)10(12)13/h1-2H,(H,8,11)(H3,7,9,1
InchiKey:	BWNXARABTNBSQF-UHFFFAOYSA-N
Formula:	C6H6N4O4S
SMILES:	NC(=S)NNC(=O)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]:	230.20
CAS:	1673-59-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	-0.334		Crippen Method
mcvol	142.790	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=C1673592&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

Latest version available from:

<https://www.chemeo.com/cid/64-960-5/Semicarbazide-1-5-nitro-2-furoyl-3-thio.pdf>

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