

Semicarbazide, 4-methyl-1-(5-nitro-2-furoyl)-3-thio-

Inchi:	InChI=1S/C7H8N4O4S/c1-8-7(16)10-9-6(12)4-2-3-5(15-4)11(13)14/h2-3H,1H3,(H,9,12)(
InchiKey:	URUMGZSJAWVTJG-UHFFFAOYSA-N
Formula:	C7H8N4O4S
SMILES:	CNC(=S)NNC(=O)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]:	244.23
CAS:	108630-85-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.33		Crippen Method
logp	-0.074		Crippen Method
mcvol	156.880	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108630859&Units=SI

Legend

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

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