

Semicarbazide, 1-(9h-purin-6-yl)-3-thio

Inchi:	InChI=1S/C6H7N7S/c7-6(14)13-12-5-3-4(9-1-8-3)10-2-11-5/h1-2H,(H3,7,13,14)(H2,8,9,1
InchiKey:	GUHAIBVGJPPBOC-UHFFFAOYSA-N
Formula:	C6H7N7S
SMILES:	NC(=S)NNc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	209.23
CAS:	25732-31-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	-0.969		Crippen Method
mcvol	138.390	ml/mol	McGowan Method

Sources

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=C25732314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/16-855-5/Semicarbazide-1-9h-purin-6-yl-3-thio.pdf>

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