

Urea, 1-[2-[9h-(purin-6-yl)thio]ethyl]-

Inchi:	InChI=1S/C8H10N6OS/c9-8(15)10-1-2-16-7-5-6(12-3-11-5)13-4-14-7/h3-4H,1-2H2,(H3,9
InchiKey:	VEILAQGIOFNDRZ-UHFFFAOYSA-N
Formula:	C8H10N6OS
SMILES:	NC(=O)NCCSc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	238.27
CAS:	90953-43-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	-0.369		Crippen Method
mcvol	162.460	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C90953438&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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