

Urea, 1-methyl-3-[2-[6-(methylthio)-9h-purin-9-yl]ethyl]-

Inchi:	InChI=1S/C10H14N6OS/c1-11-10(17)12-3-4-16-6-15-7-8(16)13-5-14-9(7)18-2/h5-6H,3-4
InchiKey:	HCSUAAPKMNZOIH-UHFFFAOYSA-N
Formula:	C10H14N6OS
SMILES:	CN=C(O)NCCn1cnc2c(SC)ncnc21
Mol. weight [g/mol]:	266.32
CAS:	90924-88-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	0.682		Crippen Method
mcvol	190.640	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=C90924882&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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