

Urea, 1-methyl-3-[2-(purin-8-ylthio)ethyl]-

Inchi:	InChI=1S/C9H12N6OS/c1-10-8(16)12-2-3-17-9-14-6-4-11-5-13-7(6)15-9/h4-5H,2-3H2,1H
InchiKey:	CKVOJWXQUZVWLC-UHFFFAOYSA-N
Formula:	C9H12N6OS
SMILES:	CNC(=O)NCCSc1nc2ncncc2[nH]1
Mol. weight [g/mol]:	252.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	-0.108		Crippen Method
mcvol	176.550	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008024&Units=SI
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

Legend

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

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