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

Inchi: InChI=1S/C9H11N7O2S/c1-16(15-18)9(17)11-2-3-19-8-13-6-4-10-5-12-7(6)14-8/h4-5H,2

InchiKey: QADBTACKEOHKRM-UHFFFAOYSA-N

Formula: C9H11N7O2S

SMILES: CN(N=O)C(=O)NCCSc1nc2ncncc2[nH]1

Mol. weight [g/mol]: 281.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	0.286		Crippen Method
mcvol	188.100	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=B6008016&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume