

Acetamide, n-[2-(9h-purin-6-yl-thio)ethyl]-

Inchi:	InChI=1S/C9H11N5OS/c1-6(15)10-2-3-16-9-7-8(12-4-11-7)13-5-14-9/h4-5H,2-3H2,1H3,(
InchiKey:	DCIFSSOGORASHV-UHFFFAOYSA-N
Formula:	C9H11N5OS
SMILES:	CC(=O)NCCSc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	237.28
CAS:	98949-69-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	0.099		Crippen Method
mcvol	166.570	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=C98949690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/60-934-8/Acetamide-n-2-9h-purin-6-yl-thio-ethyl.pdf>

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