

Purine,6-(2-aminoethyl thio)-

Inchi:	InChI=1S/C7H9N5S/c8-1-2-13-7-5-6(10-3-9-5)11-4-12-7/h3-4H,1-2,8H2,(H,9,10,11,12)
InchiKey:	RUISJPWPKNLZPR-UHFFFAOYSA-N
Formula:	C7H9N5S
SMILES:	NCCSc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	195.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	-0.078		Crippen Method
mcvol	136.820	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=B6008264&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/53-622-2/Purine-6-2-aminoethyl-thio.pdf>

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