

Ethanol, 2-[(6-amino-9h-purin-2-yl)thio]-

Inchi:	InChI=1S/C7H9N5OS/c8-5-4-6(10-3-9-4)12-7(11-5)14-2-1-13/h3,13H,1-2H2,(H3,8,9,10,11)
InchiKey:	XTHAOKUQBJUWHU-UHFFFAOYSA-N
Formula:	C7H9N5OS
SMILES:	Nc1nc(SCCO)nc2[nH]cnc12
Mol. weight [g/mol]:	211.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	-0.462		Crippen Method
mcvol	142.690	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=B6008733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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