

Ethanethiol, 2-(purin-8-yl)-

Inchi:	InChI=1S/C7H8N4S/c12-2-1-6-10-5-3-8-4-9-7(5)11-6/h3-4,12H,1-2H2,(H,8,9,10,11)
InchiKey:	SRFSTFUZPMXDOF-UHFFFAOYSA-N
Formula:	C7H8N4S
SMILES:	SCCc1nc2ncncc2[nH]1
Mol. weight [g/mol]:	180.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	0.343		Crippen Method
mcvol	126.840	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=B6008305&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

Latest version available from:

<https://www.chemeo.com/cid/13-940-3/Ethanethiol-2-purin-8-yl.pdf>

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