

4-Thiazolecarboxamide, 5-amino-2-(cyanomethylthio)-

Inchi:	InChI=1S/C6H6N4OS2/c7-1-2-12-6-10-3(4(8)11)5(9)13-6/h2,9H2,(H2,8,11)
InchiKey:	KYZWMFOIVRHOJS-UHFFFAOYSA-N
Formula:	C6H6N4OS2
SMILES:	N#CCSc1nc(C(N)=O)c(N)s1
Mol. weight [g/mol]:	214.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	0.440		Crippen Method
mcvol	141.530	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/98-613-3/4-Thiazolecarboxamide-5-amino-2-cyanomethylthio.pdf>

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