

Formamide, n-[4-amino-2,6-bis-(methylthio)-5-pyrimidinyl]-

Inchi:	InChI=1S/C7H10N4OS2/c1-13-6-4(9-3-12)5(8)10-7(11-6)14-2/h3H,1-2H3,(H,9,12)(H2,8,
InchiKey:	YLYJQBRXRIAMIN-UHFFFAOYSA-N
Formula:	C7H10N4OS2
SMILES:	CSc1nc(N)c(NC=O)c(SC)n1
Mol. weight [g/mol]:	230.31
CAS:	7595-53-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.071		Crippen Method
mcvol	159.920	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=C7595531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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