

4,5-Diamino-6-methyl-2-thiopyrimidine

Inchi:	InChI=1S/C5H8N4S/c1-2-3(6)4(7)9-5(10)8-2/h6H2,1H3,(H3,7,8,9,10)
InchiKey:	BGLOHALSDHKLSH-UHFFFAOYSA-N
Formula:	C5H8N4S
SMILES:	Cc1nc(S)[nH]c(=N)c1N
Mol. weight [g/mol]:	156.21
CAS:	6305-99-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	-0.413		Crippen Method
mcvol	113.820	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=C6305993&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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