

Pyrimidine, 2-(methylthio)-

Inchi:	InChI=1S/C5H6N2S/c1-8-5-6-3-2-4-7-5/h2-4H,1H3
InchiKey:	FOEMIZSFFWGXHX-UHFFFAOYSA-N
Formula:	C5H6N2S
SMILES:	CSc1ncccn1
Mol. weight [g/mol]:	126.18
CAS:	823-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.198		Crippen Method
mcvol	93.860	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C823096&Units=SI

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/98-420-7/Pyrimidine-2-methylthio.pdf>

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