

1H-pyrazolo(3,4-d)pyrimidine, 4-(methylthio)-

Other names:	4-(methylthio)-1H-pyrazolo[3,4-d]pyrimidine
Inchi:	InChI=1S/C6H6N4S/c1-11-6-4-2-9-10-5(4)7-3-8-6/h2-3H,1H3,(H,7,8,9,10)
InchiKey:	BLEJJILOVWBLBZ-UHFFFAOYSA-N
Formula:	C6H6N4S
SMILES:	CSc1ncnc2[nH]ncc12
Mol. weight [g/mol]:	166.20
CAS:	5418-10-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	0.593		Crippen Method
mcvol	112.750	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=C5418100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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