Pyrimidine, 4,6-dichloro-2-(methylthio)-

Other names:	4,6-Dichloro-2-methylmercaptopyrimidine
	4,6-Dichloro-2-methylthiopyrimidine
	4,6-dichloropyrimidine methyl sulphide
Inchi:	InChI=1S/C5H4Cl2N2S/c1-10-5-8-3(6)2-4(7)9-5/h2H,1H3
InchiKey:	FCMLONIWOAGZJX-UHFFFAOYSA-N
Formula:	C5H4Cl2N2S
SMILES:	CSc1nc(Cl)cc(Cl)n1
Mol. weight [g/mol]:	195.07
CAS:	6299-25-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.505		Crippen Method
mcvol	118.340	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.70	K	1.90	NIST Webbook

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=C6299258&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure