

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

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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6299258&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6299258&amp;Units=SI</a>

# Legend

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

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