

2,4-Dichloro-5-methoxypyrimidine

Inchi:	InChI=1S/C5H4Cl2N2O/c1-10-3-2-8-5(7)9-4(3)6/h2H,1H3
InchiKey:	ZTHHRSBDBPCCMZ-UHFFFAOYSA-N
Formula:	C5H4Cl2N2O
SMILES:	COc1cnc(Cl)nc1Cl
Mol. weight [g/mol]:	179.00
CAS:	19646-07-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.792		Crippen Method
mcvol	107.860	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C19646072&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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