

Pyrimidine, 4,6-dichloro-

Other names:	4,6-Dichloropyrimidine
Inchi:	InChI=1S/C4H2Cl2N2/c5-3-1-4(6)8-2-7-3/h1-2H
InchiKey:	XJPZKYIHCLDXST-UHFFFAOYSA-N
Formula:	C4H2Cl2N2
SMILES:	Clc1cc(Cl)ncn1
Mol. weight [g/mol]:	148.98
CAS:	1193-21-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.783		Crippen Method
mcvol	87.900	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.70	K	72.00	NIST Webbook

Sources

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=C1193211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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