

2,4-dichloro-5-methylpyrimidine

Other names:	5-methyl-2,4-dichloropyrimidine
Inchi:	InChI=1S/C5H4Cl2N2/c1-3-2-8-5(7)9-4(3)6/h2H,1H3
InchiKey:	DQXNTSXKIUZJJS-UHFFFAOYSA-N
Formula:	C5H4Cl2N2
SMILES:	Cc1cnc(Cl)nc1Cl
Mol. weight [g/mol]:	163.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	2.092		Crippen Method
mvol	101.990	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	64.00	kJ/mol	298.15	Thermochemical study of dichloromethylpyrimidine isomers

Sources

Thermochemical study of dichloromethylpyrimidine isomers:
McGowan Method:

<https://www.doi.org/10.1016/j.jct.2016.04.011>

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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