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
mcvol	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: https://www.doi.org/10.1016/j.jct.2016.04.011
McGowan Method: 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