

Pyrimidine, 2,4-dichloro-

Other names:	2,4-Dichloropyrimidine 2,6-Dichloropyrimidine
Inchi:	InChI=1S/C4H2Cl2N2/c5-3-1-2-7-4(6)8-3/h1-2H
InchiKey:	BTTNYQZNBZNDOR-UHFFFAOYSA-N
Formula:	C4H2Cl2N2
SMILES:	Clc1ccnc(Cl)n1
Mol. weight [g/mol]:	148.98
CAS:	3934-20-1

Physical Properties

Property code	Value	Unit	Source
hsub	76.50 ± 2.00	kJ/mol	NIST Webbook
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	374.20	K	3.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3934201&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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