

Pyrimidine, tetrachloro-

Other names:	2,4,5,6-Tetrachloro-1,3-pyrimidine 2,4,5,6-Tetrachloropyrimidine Perchloropyrimidine Pyrimidine, 2,4,5,6-tetrachloro- Tetrachloropyrimidine 2,4,5,6-Tetrachloropyrimidine
Inchi:	InChI=1S/C4Cl4N2/c5-1-2(6)9-4(8)10-3(1)7
InchiKey:	GVBHCMNXRKOJRH-UHFFFAOYSA-N
Formula:	C4Cl4N2
SMILES:	Clc1nc(Cl)c(Cl)c(Cl)n1
Mol. weight [g/mol]:	217.87
CAS:	1780-40-1

Physical Properties

Property code	Value	Unit	Source
hsub	83.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-3.74		Crippen Method
logp	3.090		Crippen Method
mvol	112.380	ml/mol	McGowan Method

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=C1780401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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