

Pyridine, pentachloro-

Other names:	2,3,4,5,6-Pentachloropyridine Pentachloropyridine Perchloropyridine Pyridine, 2,3,4,5,6-pentachloro-
Inchi:	InChI=1S/C5Cl5N/c6-1-2(7)4(9)11-5(10)3(1)8
InchiKey:	DNDPLEAVNVOOQZ-UHFFFAOYSA-N
Formula:	C5Cl5N
SMILES:	Clc1nc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	251.32
CAS:	2176-62-7

Physical Properties

Property code	Value	Unit	Source
ie	9.44	eV	NIST Webbook
log10ws	-4.66		Crippen Method
logp	4.349		Crippen Method
mcvol	128.730	ml/mol	McGowan Method
tf	397.15	K	Experimental Measurement and Correlation of Solubility of Pentachloropyridine and Tetrachloropyridine in Methanol, Ethanol, and 2-Propanol

Sources

Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Experimental Measurement and Correlation of Solubility of Pentachloropyridine and Tetrachloropyridine in Methanol, Ethanol, and 2-Propanol:	https://www.doi.org/10.1021/je0502804
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2176627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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