Pentachloropyridine

Other names:	2,3,4,5,6-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]:	251.33

Physical Properties

Property code	Value	Unit	Source
af	0.4682		Cheméo Relay (1.0)
hf	15.75	kJ/mol	Cheméo Relay (1.0)
hvap	67.89	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	NIST Webbook
log10ws	-4.81		Cheméo Relay (1.0)
logp	4.349		Crippen Method
mcvol	128.730	ml/mol	McGowan Method
pc	3615.09	kPa	Cheméo Relay (1.0, beta)
tb	550.79	K	Cheméo Relay (1.0)
tc	829.75	K	Cheméo Relay (1.0)
tf	397.15	K	Experimental Measurement and Correlation of Solubility of Pentachloropyridine and Tetrachloropyridine in Methanol, Ethanol, and 2-Propanol
vc	0.479	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Experimental Measurement and Correlation of Solubility of Pentachloropyridine and Tetrachloropyridine in Methanol, Ethanol, and 2-Propanol: https://www.doi.org/10.1021/je0502804

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2176627&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume