

3,4,5-Trichloropyridine

Inchi:	InChI=1S/C5H2Cl3N/c6-3-1-9-2-4(7)5(3)8/h1-2H
InchiKey:	KKWRVUBDCJQHBZ-UHFFFAOYSA-N
Formula:	C5H2Cl3N
SMILES:	Clc1cncc(Cl)c1Cl
Mol. weight [g/mol]:	182.44
CAS:	33216-52-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	3.042		Crippen Method
mcvol	104.250	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33216523&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/38-897-5/3-4-5-Trichloropyridine.pdf>

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