

2-(Trichloromethyl)-5-chloro pyridine

Inchi:	InChI=1S/C6H3Cl4N/c7-4-1-2-5(11-3-4)6(8,9)10/h1-3H
InchiKey:	NCMBQFDKWHROST-UHFFFAOYSA-N
Formula:	C6H3Cl4N
SMILES:	Clc1ccc(C(Cl)(Cl)Cl)nc1
Mol. weight [g/mol]:	230.91
CAS:	1197-03-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	3.562		Crippen Method
mcvol	130.580	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1197031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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