

3,5-dichloro-2-(trichloromethyl)pyridine

Other names:	3,5-Dichloro-2-trichloromethyl pyridine'
Inchi:	InChI=1S/C6H2Cl5N/c7-3-1-4(8)5(12-2-3)6(9,10)11/h1-2H
InchiKey:	PWVHFDAKFGGYKJ-UHFFFAOYSA-N
Formula:	C6H2Cl5N
SMILES:	Clc1cnc(C(Cl)(Cl)Cl)c(Cl)c1
Mol. weight [g/mol]:	265.35
CAS:	1128-16-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	4.215		Crippen Method
mcvol	142.820	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1128161&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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