

4-Amino-3,5,6-trichloro-2-(trichloromethyl)pyridin

Inchi:	InChI=1S/C6H2Cl6N2/c7-1-3(13)2(8)5(9)14-4(1)6(10,11)12/h(H2,13,14)
InchiKey:	VNJVZJNBTWPKNX-UHFFFAOYSA-N
Formula:	C6H2Cl6N2
SMILES:	Nc1c(Cl)c(Cl)nc(C(Cl)(Cl)Cl)c1Cl
Mol. weight [g/mol]:	314.81
CAS:	5005-62-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	4.451		Crippen Method
mcvol	165.040	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5005629&Units=SI

Legend

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

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