

2,4-Bis(trichloromethyl)pyridine

Inchi:	InChI=1S/C7H3Cl6N/c8-6(9,10)4-1-2-14-5(3-4)7(11,12)13/h1-3H
InchiKey:	AWCIKBIGEVDMCI-UHFFFAOYSA-N
Formula:	C7H3Cl6N
SMILES:	ClC(Cl)(Cl)c1ccnc(C(Cl)(Cl)Cl)c1
Mol. weight [g/mol]:	313.82
CAS:	6969-52-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.24		Crippen Method
logp	4.735		Crippen Method
mcvol	169.150	ml/mol	McGowan Method

Sources

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=C6969524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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