

Dibenzofuran, 1,2,3,7,8,9-hexachloro

Other names:	1,2,3,7,8,9-hexachlorodibenzofuran
Inchi:	InChI=1S/C12H2Cl6O/c13-3-1-5-7(11(17)9(3)15)8-6(19-5)2-4(14)10(16)12(8)18/h1-2H
InchiKey:	PYUSJFJVDVSXIU-UHFFFAOYSA-N
Formula:	C12H2Cl6O
SMILES:	Clc1cc2oc3cc(Cl)c(Cl)c(Cl)c3c2c(Cl)c1Cl
Mol. weight [g/mol]:	374.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.92		Crippen Method
logp	7.506		Crippen Method
mcvol	200.870	ml/mol	McGowan Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R48958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/25-717-8/Dibenzofuran-1-2-3-7-8-9-hexachloro.pdf>

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