

Dibenzofuran, 1,2,3,4,7,8,9-heptachloro

Other names:	1,2,3,4,7,8,9-heptachlorodibenzofuran
Inchi:	InChI=1S/C12HCl7O/c13-2-1-3-4(7(15)6(2)14)5-8(16)9(17)10(18)11(19)12(5)20-3/h1H
InchiKey:	VEZCTZWLJYWARH-UHFFFAOYSA-N
Formula:	C12HCl7O
SMILES:	Clc1cc2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c(Cl)c1Cl
Mol. weight [g/mol]:	409.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.61		Crippen Method
logp	8.160		Crippen Method
mcvol	213.110	ml/mol	McGowan Method
rinpol	2986.00		NIST Webbook
rinpol	2957.00		NIST Webbook
rinpol	2967.00		NIST Webbook
rinpol	2986.00		NIST Webbook

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=R29065&Units=SI

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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