

Dibenzofuran, 1,2,3,9-tetrachloro

Other names:	1,2,3,9-Tetrachlorodibenzofuran
Inchi:	InChI=1S/C12H4Cl4O/c13-5-2-1-3-7-9(5)10-8(17-7)4-6(14)11(15)12(10)16/h1-4H
InchiKey:	GNQHLJHTOATTOJ-UHFFFAOYSA-N
Formula:	C12H4Cl4O
SMILES:	Clc1cc2oc3cccc(Cl)c3c2c(Cl)c1Cl
Mol. weight [g/mol]:	305.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.55		Crippen Method
logp	6.200		Crippen Method
mcvol	176.390	ml/mol	McGowan Method
rinpol	2369.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R29172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/49-547-1/Dibenzofuran-1-2-3-9-tetrachloro.pdf>

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