

Dibenzofuran, 1,3,4,9-tetrachloro

Other names:	1,3,4,9-tetrachlorodibenzofuran
Inchi:	InChI=1S/C12H4Cl4O/c13-5-2-1-3-8-9(5)10-6(14)4-7(15)11(16)12(10)17-8/h1-4H
InchiKey:	PNCYJHOTZSKZPA-UHFFFAOYSA-N
Formula:	C12H4Cl4O
SMILES:	Clc1cc(Cl)c2c(oc3cccc(Cl)c32)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	2325.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2325.00		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=R29453&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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