

Dibenzofuran, 1,2,3,7-tetrachloro

Other names:	1,2,3,7-tetrachlorodibenzofuran
Inchi:	InChI=1S/C12H4Cl4O/c13-5-1-2-6-8(3-5)17-9-4-7(14)11(15)12(16)10(6)9/h1-4H
InchiKey:	MDNZFYGATDCKRB-UHFFFAOYSA-N
Formula:	C12H4Cl4O
SMILES:	Clc1ccc2c(c1)oc1cc(Cl)c(Cl)c(Cl)c12
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	2294.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R29140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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