

Dibenzofuran, 1,2,3,6,7-pentachloro

Other names:	1,2,3,6,7-pentachlorodibenzofuran
Inchi:	InChI=1S/C12H3Cl5O/c13-5-2-1-4-8-7(18-12(4)10(5)16)3-6(14)9(15)11(8)17/h1-3H
InchiKey:	NZUPQBVDIWCPBX-UHFFFAOYSA-N
Formula:	C12H3Cl5O
SMILES:	Clc1cc2oc3c(Cl)c(Cl)ccc3c2c(Cl)c1Cl
Mol. weight [g/mol]:	340.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.24		Crippen Method
logp	6.853		Crippen Method
mcvol	188.630	ml/mol	McGowan Method
rinpol	2522.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2557.00		NIST Webbook
rinpol	2557.00		NIST Webbook
rinpol	2540.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R29118&Units=SI
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

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/41-274-2/Dibenzofuran-1-2-3-6-7-pentachloro.pdf>

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