

Dibenzofuran, 1,2,4,7,8-pentachloro

Other names:	1,2,4,7,8-pentachlorodibenzofuran
Inchi:	InChI=1S/C12H3Cl5O/c13-5-1-4-9(3-6(5)14)18-12-8(16)2-7(15)11(17)10(4)12/h1-3H
InchiKey:	GCFDWHIKRXCUPJ-UHFFFAOYSA-N
Formula:	C12H3Cl5O
SMILES:	Clc1cc2oc3c(Cl)cc(Cl)c(Cl)c3c2cc1Cl
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	2505.00		NIST Webbook
rinpol	2473.00		NIST Webbook
rinpol	2505.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R49085&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

Latest version available from:

<https://www.chemeo.com/cid/44-943-6/Dibenzofuran-1-2-4-7-8-pentachloro.pdf>

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