

Dibenzofuran, 3,7-dichloro

Other names:	3,7-dichlorodibenzofuran
Inchi:	InChI=1S/C12H6Cl2O/c13-7-1-3-9-10-4-2-8(14)6-12(10)15-11(9)5-7/h1-6H
InchiKey:	OLTYAGNRSNFHLK-UHFFFAOYSA-N
Formula:	C12H6Cl2O
SMILES:	Clc1ccc2c(c1)oc1cc(Cl)ccc12
Mol. weight [g/mol]:	237.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.18		Crippen Method
logp	4.893		Crippen Method
mcvol	151.910	ml/mol	McGowan Method
rinpol	1930.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1925.00		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=R30054&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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