Dibenzofuran, 2,4-dichloro

Other names:	2,4-dichlorodibenzofuran
Inchi:	InChI=1S/C12H6Cl2O/c13-7-5-9-8-3-1-2-4-11(8)15-12(9)10(14)6-7/h1-6H
InchiKey:	LHTCKMYRNOGUOA-UHFFFAOYSA-N
Formula:	C12H6Cl2O
SMILES:	Clc1cc(Cl)c2oc3ccccc3c2c1
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	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1914.00		NIST Webbook

Sources

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=R29930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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