

6,8-dimethyl-1,3-dichlorodibenzofuran

Inchi:	InChI=1S/C14H10Cl2O/c1-7-3-8(2)14-10(4-7)13-11(16)5-9(15)6-12(13)17-14/h3-6H,1-2H
InchiKey:	IQULXIYKEMFITP-UHFFFAOYSA-N
Formula:	C14H10Cl2O
SMILES:	Cc1cc(C)c2oc3cc(Cl)cc(Cl)c3c2c1
Mol. weight [g/mol]:	265.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.14		Crippen Method
logp	5.510		Crippen Method
mcvol	180.090	ml/mol	McGowan Method
rinpol	2088.00		NIST Webbook
rinpol	2088.00		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=R173392&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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