

Dibenzofuran, 3,6-dichloro

Other names:	3,6-dichlorodibenzofuran
Inchi:	InChI=1S/C12H6Cl2O/c13-7-4-5-8-9-2-1-3-10(14)12(9)15-11(8)6-7/h1-6H
InchiKey:	DMOBGFAKTSXOHG-UHFFFAOYSA-N
Formula:	C12H6Cl2O
SMILES:	Clc1ccc2c(c1)oc1c(Cl)cccc12
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	1944.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1941.00		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=R30040&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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<https://www.chemeo.com/cid/28-299-0/Dibenzofuran-3-6-dichloro.pdf>

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