

Dibenzofuran, 1,3,7-trichloro

Other names:	1,3,7-trichlorodibenzofuran
Inchi:	InChI=1S/C12H5Cl3O/c13-6-1-2-8-10(4-6)16-11-5-7(14)3-9(15)12(8)11/h1-5H
InchiKey:	INRBXOGZPDFCLQ-UHFFFAOYSA-N
Formula:	C12H5Cl3O
SMILES:	Clc1ccc2c(c1)oc1cc(Cl)cc(Cl)c12
Mol. weight [g/mol]:	271.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.87		Crippen Method
logp	5.546		Crippen Method
mcvol	164.150	ml/mol	McGowan Method
rinpol	2057.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2055.00		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=R29538&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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