

Dibenzofuran, 1,2,3-trichloro

Other names:	1,2,3-trichlorodibenzofuran
Inchi:	InChI=1S/C12H5Cl3O/c13-7-5-9-10(12(15)11(7)14)6-3-1-2-4-8(6)16-9/h1-5H
InchiKey:	LADSWAAWPMGHBE-UHFFFAOYSA-N
Formula:	C12H5Cl3O
SMILES:	Clc1cc2oc3ccccc3c2c(Cl)c1Cl
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	2123.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2123.00		NIST Webbook
rinpol	2113.00		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=R29186&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

Latest version available from:

<https://www.chemeo.com/cid/85-356-3/Dibenzofuran-1-2-3-trichloro.pdf>

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