

Dibenzofuran, 3,4,8-trichloro

Other names:	3,4,8-trichlorodibenzofuran
Inchi:	InChI=1S/C12H5Cl3O/c13-6-1-4-10-8(5-6)7-2-3-9(14)11(15)12(7)16-10/h1-5H
InchiKey:	YTZWNIQGGIJHJX-UHFFFAOYSA-N
Formula:	C12H5Cl3O
SMILES:	Clc1ccc2oc3c(Cl)c(Cl)ccc3c2c1
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	2149.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2149.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2151.00		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=R30018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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