

Dibenzofuran, 3-chloro

Other names:	3-Chlorodibenzofuran
Inchi:	InChI=1S/C12H7ClO/c13-8-5-6-10-9-3-1-2-4-11(9)14-12(10)7-8/h1-7H
InchiKey:	BBOZMMAURMEVAR-UHFFFAOYSA-N
Formula:	C12H7ClO
SMILES:	Clc1ccc2c(c1)oc1cccc12
Mol. weight [g/mol]:	202.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.50		Crippen Method
logp	4.239		Crippen Method
mcvol	139.670	ml/mol	McGowan Method
rinpol	1749.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1745.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R30068&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

Latest version available from:

<https://www.cheméo.com/cid/13-095-2/Dibenzofuran-3-chloro.pdf>

Generated by Cheméo on 2024-04-27 04:06:13.90911264 +0000 UTC m=+16480022.829689951.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.