

2,3,4,6,7,8-Hexachlorodibenzofuran

Other names:	Dibenzofuran, 2,3,4,6,7,8-hexachloro-
Inchi:	InChI=1S/C12H2Cl6O/c13-5-1-3-4-2-6(14)8(16)10(18)12(4)19-11(3)9(17)7(5)15/h1-2H
InchiKey:	XTAHLACQOVXINQ-UHFFFAOYSA-N
Formula:	C12H2Cl6O
SMILES:	Clc1cc2c(oc3c(Cl)c(Cl)c(Cl)cc32)c(Cl)c1Cl
Mol. weight [g/mol]:	374.86
CAS:	60851-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.92		Crippen Method
logp	7.506		Crippen Method
mcvol	200.870	ml/mol	McGowan Method
rinpol	2748.00		NIST Webbook
rinpol	2732.00		NIST Webbook
rinpol	2737.00		NIST Webbook
rinpol	2748.00		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=C60851345&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.chemeo.com/cid/47-301-5/2-3-4-6-7-8-Hexachlorodibenzofuran.pdf>

Generated by Cheméo on 2025-12-22 19:39:05.953937955 +0000 UTC m=+6180543.483978619.

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