Dibenzofuran, octachloro-

Other names:	1,2,3,4,6,7,8,9-Octachlorodibenzo[b,d]furan
	1,2,3,4,6,7,8,9-Octachlorodibenzofuran
	Octachlorodibenzofuran
	Octapolychlorinated dibenzofuran
	Perchlorodibenzofuran
Inchi:	InChI=1S/C12Cl8O/c13-3-1-2-4(14)6(16)8(18)10(20)12(2)21-11(1)9(19)7(17)5(3)15
InchiKey:	RHIROFAGUQOFLU-UHFFFAOYSA-N
Formula:	C12Cl8O
SMILES:	Clc1c(Cl)c(Cl)c2c(oc3c(Cl)c(Cl)c(Cl)c(Cl)c32)c1Cl
Mol. weight [g/mol]:	443.75
CAS:	39001-02-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.59		Aqueous Solubility Prediction Method
logp	8.813		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
rinpol	3147.00		NIST Webbook
rinpol	3152.00		NIST Webbook
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
rinpol	3152.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	141.70 ± 1.80	kJ/mol	455.50	NIST Webbook
hsubt	149.40	kJ/mol	423.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39001020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of Selected PCDDs and PCDFs in Water and Various Chloride Solutions:	https://www.doi.org/10.1021/je700185m

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices