2,3,7,8-Tetrachlorodibenzofuran

Other names:	2,3,7,8-Tetrapolychlorinated dibenzofuran
	Dibenzofuran, 2,3,7,8-tetrachloro-
	NCI-C56611
	TCDF
Inchi:	InChI=1S/C12H4Cl4O/c13-7-1-5-6-2-8(14)10(16)4-12(6)17-11(5)3-9(7)15/h1-4H
InchiKey:	KSMVNVHUTQZITP-UHFFFAOYSA-N
Formula:	C12H4Cl4O
SMILES:	Clc1cc2oc3cc(Cl)c(Cl)cc3c2cc1Cl
Mol. weight [g/mol]:	305.97
CAS:	51207-31-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.86		Aqueous Solubility Prediction Method
logp	6.200		Crippen Method
mcvol	176.390	ml/mol	McGowan Method
rinpol	2309.00		NIST Webbook
rinpol	2338.00		NIST Webbook
rinpol	2324.00		NIST Webbook
rinpol	2342.00		NIST Webbook
rinpol	2338.00		NIST Webbook
rinpol	2309.00		NIST Webbook
rinpol	2338.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	124.00	kJ/mol	323.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C51207319&Units=SI

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