Dibenzofuran,1,2,3,4,6,7,9-heptachloro

Other names: 1,2,3,4,6,7,9-heptachlorodibenzofuran
Inchi: InChI=1S/C12HCl7O/c13-2-1-3(14)6(15)11-4(2)5-7(16)8(17)9(18)10(19)12(5)20-11/h1H
InchiKey: JWXWOEUKHXOUSK-UHFFFAOYSA-N
Formula: C12HCl7O
SMILES: Clc1cc(Cl)c2c(oc3c(Cl)c(Cl)c(Cl)c(Cl)c32)c1Cl
Mol. weight [g/mol]: 409.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.61		Crippen Method
logp	8.160		Crippen Method
mcvol	213.110	ml/mol	McGowan Method
rinpol	2913.00		NIST Webbook
rinpol	2914.00		NIST Webbook
rinpol	2913.00		NIST Webbook
rinpol	2914.00		NIST Webbook
rinpol	2913.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29015&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices