Dibenzofuran, 1,2,3,4,7,8,9-heptachloro

Other names: 1,2,3,4,7,8,9-heptachlorodibenzofuran
Inchi: InChI=1S/C12HCl7O/c13-2-1-3-4(7(15)6(2)14)5-8(16)9(17)10(18)11(19)12(5)20-3/h1H
InchiKey: VEZCTZWLJYWARH-UHFFFAOYSA-N
Formula: C12HCl7O
SMILES: Clc1cc2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c(Cl)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	2986.00		NIST Webbook
rinpol	2957.00		NIST Webbook
rinpol	2967.00		NIST Webbook
rinpol	2986.00		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=R29065&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