Dibenzofuran, octabromo

Other names:	Bibenzofuran, octabromo
	1,2,3,4,6,7,8,9-octabromo-dibenzofuran
Inchi:	InChI=1S/C12Br8O/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:	JRDWDRVPBYIYGL-UHFFFAOYSA-N
Formula:	C12Br8O
SMILES:	Brc1c(Br)c(Br)c2c(oc3c(Br)c(Br)c(Br)c(Br)c32)c1Br
Mol. weight [g/mol]:	799.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-18.12		Crippen Method
logp	9.686		Crippen Method
mcvol	267.430	ml/mol	McGowan Method
rinpol	4259.00		NIST Webbook
rinpol	4305.00		NIST Webbook
rinpol	4332.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R165990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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