1,2,3,6,7,9-hexabromo-dibenzofuran

Inchi: InChI=1S/C12H2Br6O/c13-3-1-4(14)10(17)12-7(3)8-6(19-12)2-5(15)9(16)11(8)18/h1-2H
InchiKey: YZRKGWPYPQWZHK-UHFFFAOYSA-N
Formula: C12H2Br6O
SMILES: Brc1cc2oc3c(Br)c(Br)cc(Br)c3c2c(Br)c1Br
Mol. weight [g/mol]: 641.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.79		Crippen Method
logp	8.161		Crippen Method
mcvol	232.430	ml/mol	McGowan Method
rinpol	3521.00		NIST Webbook

Sources

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=R170551&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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