1,2,3,6,7,8-hexabromo-dibenzofuran

Inchi: InChI=1S/C12H2Br6O/c13-4-1-3-7-6(2-5(14)8(15)10(7)17)19-12(3)11(18)9(4)16/h1-2H
InchiKey: VUAFSJIMHSEWBL-UHFFFAOYSA-N
Formula: C12H2Br6O
SMILES: Brc1cc2c(oc3cc(Br)c(Br)c(Br)c32)c(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	3522.00		NIST Webbook
rinpol	3522.00		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=R170531&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.