2,3,4,6,7,8-hexabromo-dibenzofuran

Inchi: InChI=1S/C12H2Br6O/c13-5-1-3-4-2-6(14)8(16)10(18)12(4)19-11(3)9(17)7(5)15/h1-2H
InchiKey: GKJPDCOZDNSVRH-UHFFFAOYSA-N
Formula: C12H2Br6O
SMILES: Brc1cc2c(oc3c(Br)c(Br)c(Br)cc32)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	3548.00		NIST Webbook
rinpol	3548.00		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=R171589&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

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