1,2,3,4,6,7,8-heptabromo-dibenzofuran

Inchi: InChI=1S/C12HBr7O/c13-3-1-2-4-6(15)7(16)8(17)10(19)12(4)20-11(2)9(18)5(3)14/h1H
InchiKey: JISOUFWSRUCDMJ-UHFFFAOYSA-N
Formula: C12HBr7O
SMILES: Brc1cc2c(oc3c(Br)c(Br)c(Br)c(Br)c32)c(Br)c1Br
Mol. weight [g/mol]: 720.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.95		Crippen Method
logp	8.924		Crippen Method
mcvol	249.930	ml/mol	McGowan Method
rinpol	3856.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R170402&Units=SI
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

Legend

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