1,2,3,6,7-pentabromo-dibenzofuran

Inchi: InChI=1S/C12H3Br5O/c13-5-2-1-4-8-7(18-12(4)10(5)16)3-6(14)9(15)11(8)17/h1-3H
InchiKey: OYKGVILGNBNCKY-UHFFFAOYSA-N
Formula: C12H3Br5O
SMILES: Brc1cc2oc3c(Br)c(Br)ccc3c2c(Br)c1Br
Mol. weight [g/mol]: 562.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.63		Crippen Method
logp	7.398		Crippen Method
mcvol	214.930	ml/mol	McGowan Method
rinpol	3164.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R170566&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