

1,2,3,4,6,7-hexabromo-dibenzofuran

Inchi: InChI=1S/C12H2Br6O/c13-4-2-1-3-5-7(15)8(16)9(17)10(18)12(5)19-11(3)6(4)14/h1-2H
InchiKey: YIOFXZCOWPMYPC-UHFFFAOYSA-N
Formula: C12H2Br6O
SMILES: BrC1ccc2c(oc3c(Br)c(Br)c(Br)c(Br)c32)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	3514.00		NIST Webbook
rinpol	3514.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R170417&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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