1,2,3,6-tetrabromo-dibenzofuran

Inchi:	InChI=1S/C12H4Br4O/c13-6-3-1-2-5-9-8(17-12(5)6)4-7(14)10(15)11(9)16/h1-4H
InchiKey:	POHZMKFDLJSOEY-UHFFFAOYSA-N
Formula:	C12H4Br4O
SMILES:	Brc1cc2oc3c(Br)cccc3c2c(Br)c1Br
Mol. weight [g/mol]:	483.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.47		Crippen Method
logp	6.636		Crippen Method
mcvol	197.430	ml/mol	McGowan Method
rinpol	2788.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R170591&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

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