

1,4,6,9-tetrabromo-dibenzofuran

Inchi:	InChI=1S/C12H4Br4O/c13-5-1-3-7(15)11-9(5)10-6(14)2-4-8(16)12(10)17-11/h1-4H
InchiKey:	GWVVZHSUINYIC-UHFFFAOYSA-N
Formula:	C12H4Br4O
SMILES:	BrC1ccc(Br)c2c1oc1c(Br)ccc(Br)c12
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	2795.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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