1,2,4-tribromo-dibenzofuran

Inchi:	InChI=1S/C12H5Br3O/c13-7-5-8(14)12-10(11(7)15)6-3-1-2-4-9(6)16-12/h1-5H
InchiKey:	GTGYFPGJRSQROX-UHFFFAOYSA-N
Formula:	C12H5Br3O
SMILES:	Brc1cc(Br)c2oc3ccccc3c2c1Br
Mol. weight [g/mol]:	404.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.30		Crippen Method
logp	5.873		Crippen Method
mcvol	179.930	ml/mol	McGowan Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R170813&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

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