

2,4,7-tribromo-dibenzofuran

Inchi:	InChI=1S/C12H5Br3O/c13-6-1-2-8-9-3-7(14)4-10(15)12(9)16-11(8)5-6/h1-5H
InchiKey:	RQIFVAZCCPQORH-UHFFFAOYSA-N
Formula:	C12H5Br3O
SMILES:	BrC1ccc2c(c1)oc1c(Br)cc(Br)cc12
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	2452.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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