

1,3,4,9-tetrabromo-dibenzofuran

Inchi:	InChI=1S/C12H4Br4O/c13-5-2-1-3-8-9(5)10-6(14)4-7(15)11(16)12(10)17-8/h1-4H
InchiKey:	KYWUFWPIZMYDJJ-UHFFFAOYSA-N
Formula:	C12H4Br4O
SMILES:	BrC1cc(Br)c2c(oc3cccc(Br)c32)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
rinpole	2803.00		NIST Webbook
rinpole	2803.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171103&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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