1,3,4,7,8-pentabromo-dibenzofuran

Inchi:	InChI=1S/C12H3Br5O/c13-5-1-4-9(3-6(5)14)18-12-10(4)7(15)2-8(16)11(12)17/h1-3H
InchiKey:	LEKZUOJYGRQREX-UHFFFAOYSA-N
Formula:	C12H3Br5O
SMILES:	Brc1cc2oc3c(Br)c(Br)cc(Br)c3c2cc1Br
Mol. weight [g/mol]:	562.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.63		Crippen Method
logp	7.398		Crippen Method
mcvol	214.930	ml/mol	McGowan Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171054&Units=SI

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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