

Dibenzofuran, 1,2,3,7,8-pentabromo

Other names:	1,2,3,7,8-pentabromo-dibenzofuran
Inchi:	InChI=1S/C12H3Br5O/c13-5-1-4-8(2-6(5)14)18-9-3-7(15)11(16)12(17)10(4)9/h1-3H
InchiKey:	QMKPILUKNSMQTD-UHFFFAOYSA-N
Formula:	C12H3Br5O
SMILES:	<chem>Brc1cc2oc3cc(Br)c(Br)c(Br)c3c2cc1Br</chem>
Mol. weight [g/mol]:	562.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.63		Crippen Method
logp	7.398		Crippen Method
mccvol	214.930	ml/mol	McGowan Method
rinpol	3145.00		NIST Webbook
rinpol	3177.00		NIST Webbook
rinpol	3180.00		NIST Webbook
rinpol	3188.00		NIST Webbook
rinpol	3204.00		NIST Webbook
rinpol	3204.00		NIST Webbook
rinpol	3145.00		NIST Webbook
rinpol	3204.00		NIST Webbook
rinpol	3182.00		NIST Webbook

Sources

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=R165985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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