Dibenzofuran, 2,3,7,8-tetrabromo-

Other names: 2,3,7,8-Tetrabromodibenzofuran
Inchi: InChI=1S/C12H4Br4O/c13-7-1-5-6-2-8(14)10(16)4-12(6)17-11(5)3-9(7)15/h1-4H
InchiKey: HCSRVQXNLHZQNM-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: Brc1cc2oc3cc(Br)c(Br)cc3c2cc1Br
Mol. weight [g/mol]: 483.78
CAS: 67733-57-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.47		Crippen Method
logp	6.636		Crippen Method
mcvol	197.430	ml/mol	McGowan Method
rinpol	2816.00		NIST Webbook
rinpol	2847.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67733577&Units=SI
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

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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