2,3,4,7-tetrabromo-dibenzofuran

Inchi: InChI=1S/C12H4Br4O/c13-5-1-2-6-7-4-8(14)10(15)11(16)12(7)17-9(6)3-5/h1-4H
InchiKey: GEXZULHQNFJAPU-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: Brc1ccc2c(c1)oc1c(Br)c(Br)c(Br)cc12
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
rinpol	2816.00		NIST Webbook
rinpol	2816.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R171643&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.