1,2,7-tribromo-dibenzofuran

Inchi: InChI=1S/C12H5Br3O/c13-6-1-2-7-10(5-6)16-9-4-3-8(14)12(15)11(7)9/h1-5H
InchiKey: IEVOJXUXBYPXKN-UHFFFAOYSA-N
Formula: C12H5Br3O
SMILES: Brc1ccc2c(c1)oc1ccc(Br)c(Br)c12
Mol. weight [g/mol]: 404.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.30		Crippen Method
logp	5.873		Crippen Method
mcvol	179.930	ml/mol	McGowan Method
rinpol	2459.00		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=R170937&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