1,3,4,7-tetrabromo-dibenzofuran

Inchi: InChI=1S/C12H4Br4O/c13-5-1-2-6-9(3-5)17-12-10(6)7(14)4-8(15)11(12)16/h1-4H
InchiKey: RUJBDWIMDZVZJI-UHFFFAOYSA-N
Formula: C12H4Br4O
SMILES: Brc1ccc2c(c1)oc1c(Br)c(Br)cc(Br)c12
Mol. weight [g/mol]: 483.78

Physical Properties

Property code	Value	Unit	Source
logp	6.636		Crippen Method
mcvol	197.430	ml/mol	McGowan Method
rinpol	2727.00		NIST Webbook
rinpol	2727.00		NIST Webbook

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R171074&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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