1,3,9-tribromo-dibenzofuran

Inchi: InChI=1S/C12H5Br3O/c13-6-4-8(15)12-10(5-6)16-9-3-1-2-7(14)11(9)12/h1-5H
InchiKey: JEOGXAUSKOAEOJ-UHFFFAOYSA-N
Formula: C12H5Br3O
SMILES: Brc1cc(Br)c2c(c1)oc1cccc(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	2466.00		NIST Webbook
rinpol	2466.00		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=R171292&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

Latest version available from:
https://www.chemeo.com/cid/83-359-2/1-3-9-tribromo-dibenzofuran.pdf
Generated by Cheméo on 2024-10-12 05:11:50.715168319 +0000 UTC m=+3290773.352137567.

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