

1,2,8-tribromo-dibenzofuran

Inchi: InChI=1S/C12H5Br3O/c13-6-1-3-9-7(5-6)11-10(16-9)4-2-8(14)12(11)15/h1-5H
InchiKey: LQKAHTKRUKHSDG-UHFFFAOYSA-N
Formula: C12H5Br3O
SMILES: BrC1ccc2oc3ccc(Br)c(Br)c3c2c1
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	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R170962&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/61-768-2/1-2-8-tribromo-dibenzofuran.pdf>

Generated by Cheméo on 2024-04-17 01:36:32.340249126 +0000 UTC m=+15607041.260826436.

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