

1,7-dibromo-dibenzofuran

Inchi: InChI=1S/C12H6Br2O/c13-7-4-5-8-11(6-7)15-10-3-1-2-9(14)12(8)10/h1-6H
InchiKey: HXTPPPWXNHSMMLZ-UHFFFAOYSA-N
Formula: C12H6Br2O
SMILES: BrC1ccc2c(c1)oc1cccc(Br)c12
Mol. weight [g/mol]: 325.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.14		Crippen Method
logp	5.111		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook

Sources

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=R171470&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/85-291-5/1-7-dibromo-dibenzofuran.pdf>

Generated by Cheméo on 2024-04-17 18:53:35.727595818 +0000 UTC m=+15669264.648173131.

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