

2,3,9-tribromo-dibenzofuran

Inchi: InChI=1S/C12H5Br3O/c13-7-2-1-3-10-12(7)6-4-8(14)9(15)5-11(6)16-10/h1-5H
InchiKey: CAJGGDCLSUA VFO-UHFFFAOYSA-N
Formula: C12H5Br3O
SMILES: Brc1cc2oc3cccc(Br)c3c2cc1Br
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	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R171801&Units=SI>
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>

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/68-521-8/2-3-9-tribromo-dibenzofuran.pdf>

Generated by Cheméo on 2025-12-06 03:00:32.816175269 +0000 UTC m=+4738230.346215924.

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