

2,4,9-tribromo-dibenzofuran

Inchi: InChI=1S/C12H5Br3O/c13-6-4-7-11-8(14)2-1-3-10(11)16-12(7)9(15)5-6/h1-5H
InchiKey: PSYFDVSLIRIJBY-UHFFFAOYSA-N
Formula: C12H5Br3O
SMILES: Brc1cc(Br)c2oc3cccc(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	2409.00		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=R171896&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/30-780-2/2-4-9-tribromo-dibenzofuran.pdf>

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