

1,2,4,6,8-pentabromo-dibenzofuran

Inchi: InChI=1S/C12H3Br5O/c13-4-1-5-9-10(17)6(14)3-8(16)12(9)18-11(5)7(15)2-4/h1-3H
InchiKey: XUMIRKPUEAOOLG-UHFFFAOYSA-N
Formula: C12H3Br5O
SMILES: BrC1cc(Br)c2oc3c(Br)cc(Br)c(Br)c3c2c1
Mol. weight [g/mol]: 562.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.63		Crippen Method
logp	7.398		Crippen Method
mcvol	214.930	ml/mol	McGowan Method
rinpol	3020.00		NIST Webbook
rinpol	3020.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R170724&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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