

1,2,3,6,7-pentabromo-dibenzofuran

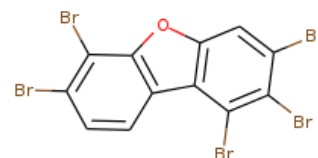
InChI: InChI=1S/C12H3Br5O/c13-5-2-1-4-8-7(18-12(4)10(5)16)3-6(14)9(15)11(8)17/h1-3H

InChI Key: OYKGVILGNBNCKY-UHFFFAOYSA-N

Formula: C12H3Br5O

SMILES: BrC1ccc2c(oc3cc(Br)c(Br)c(Br)c32)c1Br

Molecular Weight: 562.67



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	7.40		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H3Br5O/c13-5-2-1-4-8-7\(18-12\(4\)10\(5\)16\)3-6\(14\)9\(15\)11\(8\)17/h1-3H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H3Br5O/c13-5-2-1-4-8-7(18-12(4)10(5)16)3-6(14)9(15)11(8)17/h1-3H)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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