

Dibenzofuran, 3,4,7-trichloro

Other names: 3,4,7-trichlorodibenzofuran
Inchi: InChI=1S/C12H5Cl3O/c13-6-1-2-7-8-3-4-9(14)11(15)12(8)16-10(7)5-6/h1-5H
InchiKey: RPJJBTSXPNFUTA-UHFFFAOYSA-N
Formula: C12H5Cl3O
SMILES: Clc1ccc2c(c1)oc1c(Cl)c(Cl)ccc12
Mol. weight [g/mol]: 271.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.87		Crippen Method
logp	5.546		Crippen Method
mcvol	164.150	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2150.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R30004&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

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