

Dibenzofuran, 2,4,8-trichloro-

Other names: 2,4,8-trichlorodibenzofuran
Inchi: InChI=1S/C12H5Cl3O/c13-6-1-2-11-8(3-6)9-4-7(14)5-10(15)12(9)16-11/h1-5H
InchiKey: WJURXKWTCOMRCE-UHFFFAOYSA-N
Formula: C12H5Cl3O
SMILES: Clc1ccc2oc3c(Cl)cc(Cl)cc3c2c1
Mol. weight [g/mol]: 271.53
CAS: 54589-71-8

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	2099.00		NIST Webbook
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook

Sources

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=C54589718&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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<https://www.chemeo.com/cid/56-559-0/Dibenzofuran-2-4-8-trichloro.pdf>

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