

Dibenzofuran, 1,6-dichloro

Inchi: InChI=1S/C12H6Cl2O/c13-8-4-2-6-10-11(8)7-3-1-5-9(14)12(7)15-10/h1-6H
InchiKey: JRSRWACZUFLWKF-UHFFFAOYSA-N
Formula: C12H6Cl2O
SMILES: Clc1cccc2c1oc1ccc(Cl)c12
Mol. weight [g/mol]: 237.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.18		Crippen Method
logp	4.893		Crippen Method
mcvol	151.910	ml/mol	McGowan Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R49544&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/85-317-6/Dibenzofuran-1-6-dichloro.pdf>

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