Dibenzofuran, 1-chloro

Other names: 1-Chlorodibenzofuran
Inchi: InChI=1S/C12H7ClO/c13-9-5-3-7-11-12(9)8-4-1-2-6-10(8)14-11/h1-7H
InchiKey: WRSMJZYBNIAAEE-UHFFFAOYSA-N
Formula: C12H7ClO
SMILES: Clc1cccc2oc3ccccc3c12
Mol. weight [g/mol]: 202.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.50		Crippen Method
logp	4.239		Crippen Method
mcvol	139.670	ml/mol	McGowan Method
rinpol	1739.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1728.00		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=R29695&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