

2-Chloro-dibenzothiophene

Inchi: InChI=1S/C12H7ClS/c13-8-5-6-12-10(7-8)9-3-1-2-4-11(9)14-12/h1-7H
InchiKey: ZNJQWPJMTIZOHA-UHFFFAOYSA-N
Formula: C12H7ClS
SMILES: Clc1ccc2sc3ccccc3c2c1
Mol. weight [g/mol]: 218.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	4.708		Crippen Method
mcvol	150.150	ml/mol	McGowan Method
rinpol	1989.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R197021&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

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