

3-Chloro-dibenzothiophene

InChI:

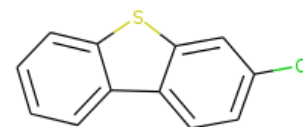
InChI=1S/C12H7ClS/c13-8-5-6-10-9-3-1-2-4-11(9)14-12(10)7-8/h1-7H

InChI Key: OTHHPAMDVKDMFM-UHFFFAOYSA-N

Formula: C12H7ClS

SMILES: Clc1ccc2c(c1)sc1cccc12

Molecular Weight: 218.70



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	4.71		Crippen Method

Sources

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H7ClS/c13-8-5-6-10-9-3-1-2-4-11\(9\)14-12\(10\)7-8/h1-7H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H7ClS/c13-8-5-6-10-9-3-1-2-4-11(9)14-12(10)7-8/h1-7H)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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