1-Chloro-dibenzothiophene

Inchi: InChI=1S/C12H7ClS/c13-9-5-3-7-11-12(9)8-4-1-2-6-10(8)14-11/h1-7H
InchiKey: UMAJBTWMRGYFLH-UHFFFAOYSA-N
Formula: C12H7ClS
SMILES: Clc1cccc2sc3ccccc3c12
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=R196964&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