

3,6-Dichloro-dibenzothiophene

Inchi: InChI=1S/C12H6Cl2S/c13-7-4-5-8-9-2-1-3-10(14)12(9)15-11(8)6-7/h1-6H
InchiKey: HYNPSGLBOMNTFF-UHFFFAOYSA-N
Formula: C12H6Cl2S
SMILES: Clc1ccc2c(c1)sc1c(Cl)cccc12
Mol. weight [g/mol]: 253.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.21		Crippen Method
logp	5.361		Crippen Method
mcvol	162.390	ml/mol	McGowan Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R197036&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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