

2,3-Dichloro-dibenzothiophene

Inchi: InChI=1S/C12H6Cl2S/c13-9-5-8-7-3-1-2-4-11(7)15-12(8)6-10(9)14/h1-6H
InchiKey: UNZMEMOIPUVLAO-UHFFFAOYSA-N
Formula: C12H6Cl2S
SMILES: Clc1cc2sc3ccccc3c2cc1Cl
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	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R196984&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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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<https://www.chemeo.com/cid/93-896-5/2-3-Dichloro-dibenzothiophene.pdf>

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