1,3-Dichloro-dibenzothiophene

Inchi: InChI=1S/C12H6Cl2S/c13-7-5-9(14)12-8-3-1-2-4-10(8)15-11(12)6-7/h1-6H
InchiKey: AVKPJBRLHOBBGI-UHFFFAOYSA-N
Formula: C12H6Cl2S
SMILES: Clc1cc(Cl)c2c(c1)sc1ccccc12
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	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R196939&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.