

2,4,8-Dichloro-dibenzothiophene

Inchi: InChI=1S/C12H5Cl3S/c13-6-1-2-11-8(3-6)9-4-7(14)5-10(15)12(9)16-11/h1-5H
InchiKey: JDABVIGRNJDKHH-UHFFFAOYSA-N
Formula: C12H5Cl3S
SMILES: Clc1ccc2sc3c(Cl)cc(Cl)cc3c2c1
Mol. weight [g/mol]: 287.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.89		Crippen Method
logp	6.015		Crippen Method
mcvol	174.630	ml/mol	McGowan Method
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R197001&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

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