1,3,6-Trichloro-dibenzothiophene

Inchi:	InChI=1S/C12H5Cl3S/c13-6-4-9(15)11-7-2-1-3-8(14)12(7)16-10(11)5-6/h1-5H
InchiKey:	VDWPANJZXVXRCC-UHFFFAOYSA-N
Formula:	C12H5Cl3S
SMILES:	Clc1cc(Cl)c2c(c1)sc1c(Cl)cccc12
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	2318.00		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=R196919&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

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