1,3,7-Trichloro-dibenzothiophene

Inchi: InChI=1S/C12H5Cl3S/c13-6-1-2-8-10(4-6)16-11-5-7(14)3-9(15)12(8)11/h1-5H
InchiKey: OHFDZAJCXMZURD-UHFFFAOYSA-N
Formula: C12H5Cl3S
SMILES: Clc1ccc2c(c1)sc1cc(Cl)cc(Cl)c12
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	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R196924&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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