Benzo[1,2-b:5,4-b']bis[1]benzothiophene

Other names: Benzo[1,2-b:5,4-b']bisthianaphthene
Inchi: InChI=1S/C18H10S2/c1-3-7-15-11(5-1)13-9-14-12-6-2-4-8-16(12)20-18(14)10-17(13)19-
InchiKey: BRSOTWFOYHMQHJ-UHFFFAOYSA-N
Formula: C18H10S2
SMILES: c1ccc2c(c1)sc1cc3sc4ccccc4c3cc12
Mol. weight [g/mol]: 290.40
CAS: 241-37-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.20		Crippen Method
logp	6.422		Crippen Method
mcvol	204.180	ml/mol	McGowan Method
rinpol	502.08		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C241372&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