9,13-H-Triphenyleno[2,3-b]thiophene

Inchi: InChI=1S/C20H12S/c1-3-7-17-15(5-1)16-6-2-4-8-18(16)20-10-14-12-21-11-13(14)9-19(1
InchiKey: KPINBESQVHNFRH-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)c1ccccc1c1cc3cscc3cc21
Mol. weight [g/mol]: 284.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.45		Crippen Method
logp	6.361		Crippen Method
mcvol	211.710	ml/mol	McGowan Method
rinpol	489.81		NIST Webbook
rinpol	489.81		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=R21055&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

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