4H-Cyclopenta[2,1-b:3,4-b']dithiophene

Inchi: InChI=1S/C9H6S2/c1-3-10-8-6(1)5-7-2-4-11-9(7)8/h1-4H,5H2
InchiKey: UITASDKJJNYORO-UHFFFAOYSA-N
Formula: C9H6S2
SMILES: c1cc2c(s1)-c1sccc1C2
Mol. weight [g/mol]: 178.27
CAS: 389-58-2

Physical Properties

Property code	Value	Unit	Source
ie	7.42	eV	NIST Webbook
log10ws	-3.94		Crippen Method
logp	3.381		Crippen Method
mcvol	120.590	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C389582&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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