Benzo[b]phenanthro[3,2-d]thiophene

Inchi: InChI=1S/C20H12S/c1-2-6-15-13(5-1)9-10-14-11-20-18(12-17(14)15)16-7-3-4-8-19(16)2
InchiKey: KBDUMZXQRUCDSI-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)ccc1cc3sc4ccccc4c3cc12
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	491.02		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=R21340&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