Benzo[b]phenanthro[9,10-d]thiophene

Inchi: InChI=1S/C20H12S/c1-3-9-15-13(7-1)14-8-2-4-10-16(14)20-19(15)17-11-5-6-12-18(17)2
InchiKey: SMDBPNFGVNKTRQ-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)sc1c3ccccc3c3ccccc3c21
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	487.32		NIST Webbook
rinpol	487.32		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21386&Units=SI
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

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.