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

Inchi: InChI=1S/C20H12S/c1-2-6-15-13(5-1)9-10-14-11-18-16-7-3-4-8-19(16)21-20(18)12-17(1
InchiKey: GDBRLJQTLSLZLH-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)ccc1cc3c(cc12)sc1ccccc13
Mol. weight [g/mol]: 284.37
CAS: 248-85-1

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	483.31		NIST Webbook
rinpol	483.31		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C248851&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