Benzo[b]phenanthro[2,1-d]thiophene

Inchi: InChI=1S/C20H12S/c1-2-6-14-13(5-1)9-10-16-15(14)11-12-19-20(16)17-7-3-4-8-18(17)2
InchiKey: XFWOYFBQPOFPRC-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)ccc1c2ccc2sc3ccccc3c21
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	487.60		NIST Webbook
rinpol	482.50		NIST Webbook
rinpol	482.20		NIST Webbook
rinpol	482.30		NIST Webbook
rinpol	487.60		NIST Webbook
rinpol	488.89		NIST Webbook
rinpol	482.30		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=R21322&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