Benzo[b]phenanthro[3,4-d]thiophene

Other names: Benzo[b]phenanthro[4,3-d]thiophene
Inchi: InChI=1S/C20H12S/c1-2-6-15-13(5-1)9-10-14-11-12-18-20(19(14)15)16-7-3-4-8-17(16)2
InchiKey: MNZURLNXWRFPND-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)ccc1ccc3sc4ccccc4c3c12
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	480.60		NIST Webbook
rinpol	467.20		NIST Webbook
rinpol	487.76		NIST Webbook
rinpol	470.47		NIST Webbook
rinpol	486.20		NIST Webbook
rinpol	481.70		NIST Webbook
rinpol	480.80		NIST Webbook
rinpol	458.50		NIST Webbook
rinpol	458.00		NIST Webbook
rinpol	480.60		NIST Webbook
rinpol	480.60		NIST Webbook
rinpol	486.20		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21368&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