Anthra[1,2-b]benzo[d]thiophene

Inchi: InChI=1S/C20H12S/c1-2-6-14-12-17-15(11-13(14)5-1)9-10-19-20(17)16-7-3-4-8-18(16)2
InchiKey: ZVPGVJPUXOINJD-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2cc3c(ccc4sc5ccccc5c43)cc2c1
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	486.70		NIST Webbook
rinpol	488.45		NIST Webbook
rinpol	482.40		NIST Webbook
rinpol	481.00		NIST Webbook
rinpol	482.40		NIST Webbook
rinpol	486.70		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21073&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