Benzo[b]phenanthro[3,2-d]thiophene, 13-methyl

Inchi: InChI=1S/C21H14S/c1-13-20-15(11-10-14-6-2-3-7-16(14)20)12-19-21(13)17-8-4-5-9-18(

InchiKey: XKKTZRYYTVHXDG-UHFFFAOYSA-N

Formula: C21H14S

SMILES: Cc1c2c(ccc3ccccc32)cc2sc3ccccc3c12

Mol. weight [g/mol]: 298.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	6.669		Crippen Method
mcvol	225.800	ml/mol	McGowan Method
rinpol	511.19		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21354&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