1-Methylphenanthro[4,5-bcd]thiophene

Other names: Phenanthro[4,5-b]thiophene, 1-methyl
Inchi: InChI=1S/C15H10S/c1-9-5-8-13-15-11(9)7-6-10-3-2-4-12(16-13)14(10)15/h2-8H,1H3
InchiKey: OMUSOOJTHCVJNY-UHFFFAOYSA-N
Formula: C15H10S
SMILES: Cc1ccc2sc3cccc4ccc1c2c43
Mol. weight [g/mol]: 222.31
CAS: 88114-01-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.53		Crippen Method
logp	4.954		Crippen Method
mcvol	165.020	ml/mol	McGowan Method
rinpol	371.20		NIST Webbook

Sources

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=C88114016&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices