Triphenyleno[4,5-bcd]thiophene

Other names: Triphenyleno[1,12-bcd]thiophene
Inchi: InChI=1S/C18H10S/c1-2-6-12-11(5-1)13-7-3-9-15-17(13)18-14(12)8-4-10-16(18)19-15/h
InchiKey: GFFHWBASMBTYKN-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1ccc2c(c1)c1cccc3sc4cccc2c4c31
Mol. weight [g/mol]: 258.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	5.799		Crippen Method
mcvol	187.830	ml/mol	McGowan Method
rinpol	448.50		NIST Webbook
rinpol	447.99		NIST Webbook
rinpol	439.00		NIST Webbook
rinpol	447.99		NIST Webbook
rinpol	448.50		NIST Webbook
rinpol	448.10		NIST Webbook
rinpol	448.45		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21792&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