Benzo[1,2]phenaleno[4,3-bc]thiophene

Inchi: InChI=1S/C18H10S/c1-2-6-13-12(5-1)14-7-3-4-11-8-9-16-18(17(11)14)15(13)10-19-16/h
InchiKey: KQBTZZAHVTXQQK-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1ccc2c(c1)c1cccc3ccc4scc2c4c31
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	482.99		NIST Webbook
rinpol	466.40		NIST Webbook
rinpol	466.60		NIST Webbook
rinpol	472.90		NIST Webbook
rinpol	472.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21112&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