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

Inchi: InChI=1S/C18H10S/c1-2-6-15-13(5-1)14-7-3-4-11-8-9-12-10-19-18(15)17(12)16(11)14/h
InchiKey: KUXSKRKPJSNSLI-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1ccc2c(c1)c1cccc3ccc4csc2c4c31
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	447.85		NIST Webbook
rinpol	447.85		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21108&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.