Benzo[2,3]phenanthro[4,5]thiophene, 1-methyl

Inchi: InChI=1S/C19H12S/c1-11-6-7-12-8-9-14-10-13-4-2-3-5-15(13)19-17(14)16(12)18(11)20-

InchiKey: DPTVXLZSFDBXBV-UHFFFAOYSA-N

Formula: C19H12S

SMILES: Cc1ccc2ccc3cc4ccccc4c4sc1c2c34

Mol. weight [g/mol]: 272.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	6.107		Crippen Method
mcvol	201.920	ml/mol	McGowan Method
rinpol	452.67		NIST Webbook
rinpol	452.67		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R642492&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.