acenaphtho[4,3-b]benzo[d]thiophene

Inchi: InChI=1S/C18H12S/c1-2-7-15-13(6-1)18-14-9-8-11-4-3-5-12(17(11)14)10-16(18)19-15/h
InchiKey: JKSVSYMOAXIDQO-UHFFFAOYSA-N
Formula: C18H12S
SMILES: c1cc2c3c(c4c(cc3c1)sc1ccccc14)CC2
Mol. weight [g/mol]: 260.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	5.306		Crippen Method
mcvol	192.130	ml/mol	McGowan Method
rinpol	456.18		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R197690&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