Acenaphthyleno[4,5-a]dibenzothiophene

Inchi: InChI=1S/C22H12S/c1-2-7-18-16(5-1)22-19(23-18)11-10-15-12-14-9-8-13-4-3-6-17(20(1

InchiKey: OWRNZBTXMZTPQY-UHFFFAOYSA-N

Formula: C22H12S

SMILES: C1=Cc2cc3ccc4sc5ccccc5c4c3c3cccc1c23

Mol. weight [g/mol]: 308.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.30		Crippen Method
logp	6.845		Crippen Method
mcvol	224.730	ml/mol	McGowan Method
rinpol	536.75		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R642432&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