

Pyreno[2,1-b]thiophene

Inchi: InChI=1S/C18H10S/c1-2-11-4-5-13-10-16-14(8-9-19-16)15-7-6-12(3-1)17(11)18(13)15/h
InchiKey: KBGGQFXYUZPGSX-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1cc2ccc3cc4sccc4c4ccc(c1)c2c34
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	455.50		NIST Webbook
rinpol	455.14		NIST Webbook
rinpol	455.01		NIST Webbook
rinpol	446.20		NIST Webbook
rinpol	446.40		NIST Webbook
rinpol	446.60		NIST Webbook
rinpol	446.20		NIST Webbook
rinpol	455.50		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R21742&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

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