

Pyreno[1,2-b]thiophene

Inchi:	InChI=1S/C18H10S/c1-2-11-4-5-13-10-14-8-9-19-18(14)15-7-6-12(3-1)16(11)17(13)15/h
InchiKey:	KCKFFTQULGAQPQ-UHFFFAOYSA-N
Formula:	C18H10S
SMILES:	<chem>c1cc2ccc3cc4ccsc4c4ccc(c1)c2c34</chem>
Mol. weight [g/mol]:	258.34
CAS:	189-83-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	5.799		Crippen Method
mccvol	187.830	ml/mol	McGowan Method
rinpol	450.00		NIST Webbook
rinpol	449.56		NIST Webbook
rinpol	449.30		NIST Webbook
rinpol	440.70		NIST Webbook
rinpol	441.10		NIST Webbook
rinpol	441.30		NIST Webbook
rinpol	441.30		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	441.30		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C189833&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
mcpol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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