Phenanthro[4,5-b]thiophene

Inchi:	InChI=1S/C14H8S/c1-3-9-7-8-10-4-2-6-12-14(10)13(9)11(5-1)15-12/h1-8H
InchiKey:	VFUBXBLVICASPS-UHFFFAOYSA-N
Formula:	C14H8S
SMILES:	c1cc2ccc3cccc4sc(c1)c2c34
Mol. weight [g/mol]:	208.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	4.646		Crippen Method
mcvol	150.930	ml/mol	McGowan Method
rinpol	349.65		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R643099&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

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