

Phenanthro[4,5-bcd]thiophene

Other names:	[4,5-bcd]phenanthrothiophene Phenanthro[4.5-bcd]thiophene Phenanthro[4,5-bcd]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:	<chem>c1cc2ccc3cccc4sc(c1)c2c34</chem>
Mol. weight [g/mol]:	208.28
CAS:	30796-92-0

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	349.42		NIST Webbook
rinpol	349.17		NIST Webbook
rinpol	349.42		NIST Webbook
rinpol	350.00		NIST Webbook
rinpol	349.17		NIST Webbook
rinpol	348.75		NIST Webbook
rinpol	2067.10		NIST Webbook
rinpol	349.17		NIST Webbook
rinpol	349.42		NIST Webbook
rinpol	350.00		NIST Webbook
rinpol	348.85		NIST Webbook
rinpol	348.20		NIST Webbook
rinpol	348.20		NIST Webbook
rinpol	348.75		NIST Webbook
rinpol	347.89		NIST Webbook
rinpol	2067.10		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30796920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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