

1-Thia-6-selenacyclodeca-3,8-diyne

Inchi:	InChI=1S/C8H8SSe/c1-3-7-10-8-4-2-6-9-5-1/h5-8H2
InchiKey:	GFFMWKZLVLEU-UHFFFAOYSA-N
Formula:	C8H8SSe
SMILES:	C1#CC[Se]CC#CCSC1
Mol. weight [g/mol]:	215.17
CAS:	127793-17-3

Physical Properties

Property code	Value	Unit	Source
ie	8.20	eV	NIST Webbook
ie	8.39	eV	NIST Webbook
log10ws	-0.08		Crippen Method
logp	1.281		Crippen Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127793173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/56-839-9/1-Thia-6-selenacyclodeca-3-8-diyne.pdf>

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