

1-Oxa-6-thiacyclodeca-3,8-diyne

Inchi: InChI=1S/C8H8OS/c1-3-7-10-8-4-2-6-9-5-1/h5-8H2
InchiKey: NENVKWPSERARAT-UHFFFAOYSA-N
Formula: C8H8OS
SMILES: C1#CCSCC#CCOC1
Mol. weight [g/mol]: 152.21
CAS: 127793-16-2

Physical Properties

Property code	Value	Unit	Source
ie	8.70	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
log10ws	-1.63		Crippen Method
logp	0.757		Crippen Method
mcvol	117.740	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C127793162&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

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/52-764-6/1-Oxa-6-thiacyclodeca-3-8-diyne.pdf>

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