Oxacyclotetradeca-4,11-diyne

Other names:	Oxacyclotetradeca-4,11-dyine
Inchi:	InChI=1S/C13H18O/c1-2-4-6-8-10-12-14-13-11-9-7-5-3-1/h1-5,10-13H2
InchiKey:	ISEQOSOYOGJYOG-UHFFFAOYSA-N
Formula:	C13H18O
SMILES:	C1#CCCOCCC#CCCCCC1
Mol. weight [g/mol]:	190.28
CAS:	6568-32-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.754		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6568327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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