

Sesquirosefuran

Other names:	(E)-2-(3,7-dimethylocta-2,6-dien-1-yl)-3-methylfuran
Inchi:	InChI=1S/C15H22O/c1-12(2)6-5-7-13(3)8-9-15-14(4)10-11-16-15/h6,8,10-11H,5,7,9H2,1
InchiKey:	CKUQXDUZAWSPOV-MDWZMJQESA-N
Formula:	C15H22O
SMILES:	CC(C)=CCCC(C)=CCc1occc1C
Mol. weight [g/mol]:	218.33
CAS:	39007-93-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.54		Crippen Method
logp	4.823		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
rinpol	1557.10		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1557.10		NIST Webbook
rinpol	1549.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39007937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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