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