

Furan, 2-methyl-5-(1,1,5-trimethyl-5-hexenyl)-

Other names: Furane-2-methyl-5-(1,1,5-trimethyl-5-hexenyl)
Inchi: InChI=1S/C14H22O/c1-11(2)7-6-10-14(4,5)13-9-8-12(3)15-13/h8-9H,1,6-7,10H2,2-5H3
InchiKey: GHWXKPRRVHJBAE-UHFFFAOYSA-N
Formula: C14H22O
SMILES: C=C(C)CCCC(C)(C)c1ccc(C)o1
Mol. weight [g/mol]: 206.32
CAS: 77143-15-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	4.612		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
rinpol	1458.00		NIST Webbook
rinpol	1440.00		NIST Webbook
ripol	1956.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C77143158&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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