Ethanone, 1-[3-[2-methyl-2-(5-methyl-2-furanyl)propyl]oxiran

Other names: 1-[3-[2-Methyl-2-[5-methyl-2-furanyl]propyl]oxiranyl]-ethanone
Inchi: InChI=1S/C13H18O3/c1-8-5-6-11(15-8)13(3,4)7-10-12(16-10)9(2)14/h5-6,10,12H,7H2,1-
InchiKey: NRYBNWWOESXFHO-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CC(=O)C1OC1CC(C)(C)c1ccc(C)o1
Mol. weight [g/mol]: 222.28
CAS: 80114-28-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	2.612		Crippen Method
mcvol	177.020	ml/mol	McGowan Method
ripol	1979.00		NIST Webbook
ripol	1979.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80114289&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

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

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