1-((1R,2R,3R)-2-(3-Isopropylfuran-2-yl)-3-methylcy

Other names:	Ethanone, 1-[(1R,2R,3R)-3-methyl-2-[3-(1-methylethyl)-2-furanyl]cyclopentyl]-
	Ethanone, 1-[3-methyl-2-[3-(1-methylethyl)-2-furanyl]cyclopentyl]-, [1R-(1«alpha»,2«beta»,3«beta»)]-
	Furopelargone A
	furopelargone
Inchi:	InChI=1S/C15H22O2/c1-9(2)12-7-8-17-15(12)14-10(3)5-6-13(14)11(4)16/h7-10,13-14H,5
InchiKey:	DVIZGXBTTFXQQC-DDTOSNHZSA-N
Formula:	C15H22O2
SMILES:	CC(=O)C1CCC(C)C1c1occc1C(C)C
Mol. weight [g/mol]:	234.33
CAS:	1143-45-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.36		Crippen Method
logp	4.122		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
rinpol	1588.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1143459&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

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