2-Octalen-1-one, 3,4a,8,8-tetramethyl, 4-(2-(3-furyl)ethyl))

Inchi: InChI=1S/C20H28O2/c1-14-12-17(21)18-19(2,3)9-5-10-20(18,4)16(14)7-6-15-8-11-22-13

InchiKey: ADPXGTXMLRWKFG-UHFFFAOYSA-N

Formula: C20H28O2

SMILES: CC1=CC(=O)C2C(C)(C)CCCC2(C)C1CCc1ccoc1

Mol. weight [g/mol]: 300.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.82		Crippen Method
logp	5.190		Crippen Method
mcvol	254.620	ml/mol	McGowan Method
rinpol	2089.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R399425&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

rinpol: Non-polar retention indices