6-Methyl-6-(5-methylfuran-2-yl)heptan-2-one

Inchi: InChI=1S/C13H20O2/c1-10(14)6-5-9-13(3,4)12-8-7-11(2)15-12/h7-8H,5-6,9H2,1-4H3
InchiKey: CQPPRTJQWXGAGK-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC(=O)CCCC(C)(C)c1ccc(C)o1
Mol. weight [g/mol]: 208.30
CAS: 50464-95-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	3.625		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
rinpol	1426.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1426.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50464954&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

Latest version available from: