1-(Furan-2-yl)-4-methylpentan-1-one

Inchi: InChI=1S/C10H14O2/c1-8(2)5-6-9(11)10-4-3-7-12-10/h3-4,7-8H,5-6H2,1-2H3
InchiKey: SCZPAWWSCDSDKR-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC(C)CCC(=O)c1ccco1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	2.898		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1253.00		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=U412814&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