

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

Inchi: InChI=1S/C10H14O2/c1-3-5-8(2)10(11)9-6-4-7-12-9/h4,6-8H,3,5H2,1-2H3
InchiKey: ZONAONHRDHDNFB-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CCCC(C)C(=O)c1ccco1
Mol. weight [g/mol]: 166.22
CAS: 1248070-62-3

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	1267.90		NIST Webbook
rinpol	1267.90		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C1248070623&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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