

5-(Furan-3-yl)-2-methylpent-1-en-3-one

Inchi:	InChI=1S/C10H12O2/c1-8(2)10(11)4-3-9-5-6-12-7-9/h5-7H,1,3-4H2,2H3
InchiKey:	XUCQQLCBOJJVRF-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	C=C(C)C(=O)CCc1ccoc1
Mol. weight [g/mol]:	164.20
CAS:	80445-58-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	2.357		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
rinpol	1259.10		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80445585&Units=SI
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

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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