3-Penten-2-one, 3-(2-furanyl)-

Other names: 3-(2-Furyl)-3-penten-2-one
3-(2-Furanyl)-3-penten-2-one
Inchi: InChI=1S/C9H10O2/c1-3-8(7(2)10)9-5-4-6-11-9/h3-6H,1-2H3/b8-3+
InchiKey: JXBNWSXFXIUPHP-FPYGCLRLSA-N
Formula: C9H10O2
SMILES: CC=C(C(C)=O)c1ccco1
Mol. weight [g/mol]: 150.17
CAS: 56335-77-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.56		Crippen Method
logp	2.272		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
ripol	1933.00		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=C56335774&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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