1-(5-methy1-2-furanyl)-1-buten-3-one

Other names: 1-(5-methyl-2-furanyl)-1-buten-3-one
Inchi: InChI=1S/C9H10O2/c1-7(10)3-5-9-6-4-8(2)11-9/h3-6H,1-2H3/b5-3+
InchiKey: FKNBELIGEMXLJS-HWKANZROSA-N
Formula: C9H10O2
SMILES: CC(=O)C=Cc1ccc(C)o1
Mol. weight [g/mol]: 150.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	2.190		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
ripol	1990.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1992.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1990.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1990.00		NIST Webbook
ripol	1949.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R296658&Units=SI
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

Legend

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