2-Butanone, 4-(5-methyl-2-furanyl)-

Other names:	4-(5-Methyl-2-furyl)-2-butanone
	Furan, 2-methyl-5-(3-oxobutyl)
	1-(5-methyl-2-furanyl)-3-butanone
	2-Butanone, 4-(5-methyl-2-furyl)
	4-(5-Methyl-2-furanyl)-2-butanone
Inchi:	InChI=1S/C9H12O2/c1-7(10)3-5-9-6-4-8(2)11-9/h4,6H,3,5H2,1-2H3
InchiKey:	CWKYCXPGVIFXOH-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CC(=O)CCc1ccc(C)o1
Mol. weight [g/mol]:	152.19
CAS:	13679-56-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	2.110		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1709.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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