trans-(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	1992.00		NIST Webbook
ripol	1992.00		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=R492896&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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