1-(5-methy1-2-furanyl)-1-propen-3-al

Inchi: InChI=1S/C8H8O2/c1-7-4-5-8(10-7)3-2-6-9/h2-6H,1H3/b3-2+
InchiKey: XYYLGSWUPMPWLD-NSCUHMNNSA-N
Formula: C8H8O2
SMILES: Cc1ccc(C=CC=O)o1
Mol. weight [g/mol]: 136.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.20		Crippen Method
logp	1.800		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
ripol	1855.00		NIST Webbook
ripol	1855.00		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=R296663&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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