

1-(5-hydroxymethyl-2-furanyl)-propanone

Inchi:	InChI=1S/C8H10O3/c1-2-7(10)8-4-3-6(5-9)11-8/h3-4,9H,2,5H2,1H3
InchiKey:	RMCCJYHRLNRZNJ-UHFFFAOYSA-N
Formula:	C8H10O3
SMILES:	CCC(=O)c1ccc(CO)o1
Mol. weight [g/mol]:	154.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	1.365		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
ripol	2599.00		NIST Webbook
ripol	2599.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/81-355-8/1-5-hydroxymethyl-2-furanyl-propanone.pdf>

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