5-Acetyl-2-furanmethanol

Other names:	1-(5-hydroxymethyl-2-furanyl)-ethanone
Inchi:	InChI=1S/C7H8O3/c1-5(9)7-3-2-6(4-8)10-7/h2-3,8H,4H2,1H3
InchiKey:	WPUGXTIOWBWKJY-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	CC(=O)c1ccc(CO)o1
Mol. weight [g/mol]:	140.14
CAS:	55087-82-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	0.975		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
ripol	2542.00		NIST Webbook
ripol	2519.00		NIST Webbook

Sources

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=C55087826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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