Furyl hydroxymethyl ketone

Other names:	Ethanone, 1-(2-furanyl)-2-hydroxy-
	Ketone, 2-furyl hydroxymethyl
	2-(Hydroxyacetyl)furan
	2-Furyl hydroxymethyl ketone
	2-(2'-Hydroxyacetyl)furan
	2-(1-Oxo-2-hydroxyethyl)furan
	1-(2furyl)-2-hydroxyethanone
Inchi:	InChI=1S/C6H6O3/c7-4-5(8)6-2-1-3-9-6/h1-3,7H,4H2
InchiKey:	RSZZMVPSHLKFQY-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	O=C(CO)c1ccco1
Mol. weight [g/mol]:	126.11
CAS:	17678-19-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	0.455		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	1087.00		NIST Webbook
rinpol	1086.30		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1086.30		NIST Webbook
ripol	2001.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	2001.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	1989.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17678192&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