

2(5H)-Furanone, 5-(2-furanylmethyl)-5-methyl-

Other names:	2(5H)-Furanone, 5-furfuryl-5-methyl- 4-Furfuyl-3-hydroxy-2-pentenoic acid «gamma»-lactone 5-Methyl-5-furfuryl-2(5H)-furanone
Inchi:	InChI=1S/C10H10O3/c1-10(5-4-9(11)13-10)7-8-3-2-6-12-8/h2-6H,7H2,1H3
InchiKey:	BJDSCPMXFWDFDR-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CC1(Cc2ccco2)C=CC(=O)O1
Mol. weight [g/mol]:	178.18
CAS:	31969-27-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	1.694		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
ripol	2311.00		NIST Webbook
ripol	2311.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31969274&Units=SI
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

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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