2-Furanmethanol, propanoate

Other names:	Furfuryl alcohol, propionate
	Furfuryl propionate
	2-furfuryl propanoate
	Furfuryl alcohol propanoate
	furfuryl-propanoate
Inchi:	InChI=1S/C8H10O3/c1-2-8(9)11-6-7-4-3-5-10-7/h3-5H,2,6H2,1H3
InchiKey:	LGBXNZSSTFWRFS-UHFFFAOYSA-N
Formula:	C8H10O3
SMILES:	CCC(=O)OCc1ccco1
Mol. weight [g/mol]:	154.16
CAS:	623-19-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.20		Crippen Method
logp	1.733		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1096.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1583.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623198&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