Furfuryl formate

Other names:	2-Furylmethyl formate
	Furfuryl methanoate
	2-Furanmethanol, 2-formate
	furan-2-ylmethyl formate
Inchi:	InChI=1S/C6H6O3/c7-5-8-4-6-2-1-3-9-6/h1-3,5H,4H2
InchiKey:	FPRQARNPKWVCNI-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	O=COCc1ccco1
Mol. weight [g/mol]:	126.11
CAS:	13493-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	0.953		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	902.00		NIST Webbook
rinpol	875.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1519.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13493975&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