Furfuryl hexanoate

Other names:	Furfuryl n-hexanoate
	Hexanoic acid, 2-furanylmethyl ester
	furan-2-ylmethyl hexanoate
Inchi:	InChI=1S/C11H16O3/c1-2-3-4-7-11(12)14-9-10-6-5-8-13-10/h5-6,8H,2-4,7,9H2,1H3
InchiKey:	IBIDUABZZSJJNF-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	CCCCCC(=O)OCc1ccco1
Mol. weight [g/mol]:	196.24
CAS:	39252-02-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.46		Crippen Method
logp	2.903		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
rinpol	1368.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1343.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1850.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39252023&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