Furfuryl heptanoate

Other names:	Heptanoic acid, 2-furanylmethyl ester
	furan-2-ylmethyl heptanoate
Inchi:	InChI=1S/C12H18O3/c1-2-3-4-5-8-12(13)15-10-11-7-6-9-14-11/h6-7,9H,2-5,8,10H2,1H3
InchiKey:	VZRGLBPRLIGTPE-UHFFFAOYSA-N
Formula:	C12H18O3
SMILES:	CCCCCCC(=O)OCc1ccco1
Mol. weight [g/mol]:	210.27
CAS:	39481-28-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.88		Crippen Method
logp	3.293		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
rinpol	1443.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1950.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39481282&Units=SI

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

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