

Furfuryl pentanoate

Other names:	Pentanoic acid, 2-furanylmethyl ester Furfuryl valerate
Inchi:	InChI=1S/C10H14O3/c1-2-3-6-10(11)13-8-9-5-4-7-12-9/h4-5,7H,2-3,6,8H2,1H3
InchiKey:	HRYAVTBTUKVHBU-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CCCCC(=O)OCc1ccco1
Mol. weight [g/mol]:	182.22
CAS:	36701-01-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.04		Crippen Method
logp	2.513		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
ripol	1753.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36701016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices

ripol: Polar retention indices

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