2-Furancarboxylic acid, 3-methylbutyl ester

Other names:	iso-Amyl 2-furoate
	Isoamyl furoate
	2-Furoic acid, 3-methylbutyl ester
	3-methylbutyl 2-furoate
Inchi:	InChI=1S/C10H14O3/c1-8(2)5-7-13-10(11)9-4-3-6-12-9/h3-4,6,8H,5,7H2,1-2H3
InchiKey:	FPBZWZKAUPNMMV-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CC(C)CCOC(=O)c1ccco1
Mol. weight [g/mol]:	182.22
CAS:	615-12-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.88		Crippen Method
logp	2.482		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1287.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1840.00		NIST Webbook

Sources

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=C615123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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