Furfuryl isovalerate

Other names:	Furfuryl 3-methylbutanoate
	Furfuryl isovalerate
Inchi:	InChI=1S/C10H14O3/c1-8(2)6-10(11)13-7-9-4-3-5-12-9/h3-5,8H,6-7H2,1-2H3
InchiKey:	FKGUIBCHHSHJNQ-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CC(C)CC(=O)OCc1ccco1
Mol. weight [g/mol]:	182.22

Physical Properties

Property code	Value	Unit	Source
hf	-479.77	kJ/mol	Cheméo Relay (1.0)
hvap	58.11	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
logp	2.369		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1223.70		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1222.00		NIST Webbook
tb	466.47	K	Cheméo Relay (1.0)
tc	689.35	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13678609&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature