iso-Amyl furylpropionate

Other names: 3-methylbutyl furan-2-propionate
iso-Amyl furylpropionate
Inchi: InChI=1S/C12H18O3/c1-10(2)7-9-15-12(13)6-5-11-4-3-8-14-11/h3-4,8,10H,5-7,9H2,1-2H
InchiKey: ZVMWAVZRUZDYMV-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: CC(C)CCOC(=O)CCc1ccco1
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
hf	-530.39	kJ/mol	Cheméo Relay (1.0)
hvap	67.14	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.68		Cheméo Relay (1.0)
logp	2.801		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
tb	531.77	K	Cheméo Relay (1.0)
tc	715.58	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=C7779671&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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