(S)-Isopropyl lactate

Other names:	isopropyl (S)-(-)-lactate
	isopropyl (S)-2-hydroxypropionate
	isopropyl (S)-lactate
	isopropyl S-(-)-lactate
	propanoic acid, 2-hydroxy-, 1-methylethyl ester, (S)-
Inchi:	InChI=1S/C6H12O3/c1-4(2)9-6(8)5(3)7/h4-5,7H,1-3H3/t5-/m1/s1
InchiKey:	KIWATKANDHUUOB-RXMQYKEDSA-N
Formula:	C6H12O3
SMILES:	CC(C)OC(=O)C(C)O
Mol. weight [g/mol]:	132.16
CAS:	63697-00-7

Physical Properties

Property code	Value	Unit	Source
gf	-375.98	kJ/mol	Joback Method
hf	-574.76	kJ/mol	Joback Method
hfus	11.12	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	0.319		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	504.27	K	Joback Method
tc	682.14	K	Joback Method
tf	260.36	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.77	J/mol×K	682.14	Joback Method
cpg	246.04	J/mol×K	504.27	Joback Method
cpg	255.38	J/mol×K	533.92	Joback Method
cpg	264.36	J/mol×K	563.56	Joback Method

cpg	272.99	J/mol×K	593.21	Joback Method
cpg	281.27	J/mol×K	622.85	Joback Method
cpg	289.19	J/mol×K	652.50	Joback Method
dvisc	0.0001409	Pa×s	504.27	Joback Method
dvisc	0.0398736	Pa×s	260.36	Joback Method
dvisc	0.0082434	Pa×s	301.01	Joback Method
dvisc	0.0024799	Pa×s	341.66	Joback Method
dvisc	0.0009632	Pa×s	382.31	Joback Method
dvisc	0.0004487	Pa×s	422.97	Joback Method
dvisc	0.0002390	Pa×s	463.62	Joback Method
pvap	0.41	kPa	306.80	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.09	kPa	283.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.12	kPa	288.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.18	kPa	293.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.24	kPa	298.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.32	kPa	303.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
rfi	1.41050		293.15	Vapor liquid equilibria and excess volumes of the binary systems ethanol + ethyl lactate, isopropanol + isopropyl lactate and n-butanol + n-butyl lactate at 101.325 kPa

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63697007&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor liquid equilibria and excess volumes of the binary systems ethanol + ethyl lactate, isopropanol + isopropyl lactate and n-butanol + n-butyl lactate at 101.325 kPa:	https://www.doi.org/10.1016/j.fluid.2005.02.015
Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.jct.2018.07.029
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume