

(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/molxK	682.14	Joback Method
cpg	246.04	J/molxK	504.27	Joback Method
cpg	255.38	J/molxK	533.92	Joback Method
cpg	264.36	J/molxK	563.56	Joback Method

cpg	272.99	J/molxK	593.21	Joback Method
cpg	281.27	J/molxK	622.85	Joback Method
cpg	289.19	J/molxK	652.50	Joback Method
dvisc	0.0001409	Paxs	504.27	Joback Method
dvisc	0.0398736	Paxs	260.36	Joback Method
dvisc	0.0082434	Paxs	301.01	Joback Method
dvisc	0.0024799	Paxs	341.66	Joback Method
dvisc	0.0009632	Paxs	382.31	Joback Method
dvisc	0.0004487	Paxs	422.97	Joback Method
dvisc	0.0002390	Paxs	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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

Legend

cp _g :	Ideal gas heat capacity
dv _{isc} :	Dynamic viscosity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
p_{vap}:	Vapor pressure
r_{fi}:	Refractive Index
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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