

# Propanoic acid, 2-hydroxy-, ethyl ester, (L)-

Other names:	(+)-ethyl lactate (R)-(+)-ethyl lactate D-ethyl lactate Ethyl (L)-(-)-lactate Ethyl (S)-(-)-lactate Ethyl 2-hydroxypropanoate, (L)- Propanoic acid, 2-hydroxy-, ethyl ester, (S)- ethyl (R)-2-hydroxypropanoate ethyl (R)-2-hydroxypropionate ethyl (S)-2-hydroxypropionate ethyl D-lactate
Inchi:	InChI=1S/C5H10O3/c1-3-8-5(7)4(2)6/h4,6H,3H2,1-2H3/t4-/m1/s1
InchiKey:	LZCLXQDLBQLTDK-SCSAIBSYSA-N
Formula:	C5H10O3
SMILES:	CCOC(=O)C(C)O
Mol. weight [g/mol]:	118.13
CAS:	687-47-8

## Physical Properties

Property code	Value	Unit	Source
gf	-381.96	kJ/mol	Joback Method
hf	-548.84	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.070		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
ripol	1356.00		NIST Webbook
tb	427.25 ± 0.50	K	NIST Webbook
tb	427.10 ± 0.50	K	NIST Webbook
tb	427.10 ± 0.50	K	NIST Webbook
tb	427.10 ± 0.50	K	NIST Webbook
tb	427.20	K	NIST Webbook
tc	657.66	K	Joback Method
tf	264.09	K	Joback Method
vc	0.352	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.43	J/molxK	657.66	Joback Method
cpg	212.77	J/molxK	511.13	Joback Method
cpg	220.46	J/molxK	540.44	Joback Method
cpg	227.87	J/molxK	569.74	Joback Method
cpg	235.00	J/molxK	599.05	Joback Method
cpg	241.86	J/molxK	628.35	Joback Method
cpg	204.80	J/molxK	481.83	Joback Method
dvisc	0.0002891	Paxs	445.54	Joback Method
dvisc	0.0005156	Paxs	409.25	Joback Method
dvisc	0.0010292	Paxs	372.96	Joback Method
dvisc	0.0023843	Paxs	336.67	Joback Method
dvisc	0.0067671	Paxs	300.38	Joback Method
dvisc	0.0001769	Paxs	481.83	Joback Method
dvisc	0.0255824	Paxs	264.09	Joback Method
pvap	0.11	kPa	286.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.14	kPa	289.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.16	kPa	291.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.19	kPa	293.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.21	kPa	295.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.26	kPa	297.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.28	kPa	298.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.10	kPa	285.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.29	kPa	299.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.35	kPa	301.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.39	kPa	303.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.46	kPa	305.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.48	kPa	306.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.52	kPa	307.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.56	kPa	308.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.58	kPa	308.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.65	kPa	310.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.70	kPa	311.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.76	kPa	313.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.81	kPa	314.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.95	kPa	316.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	1.05	kPa	318.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.08	kPa	283.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.08	kPa	282.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.07	kPa	280.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.06	kPa	278.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.05	kPa	276.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.04	kPa	274.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.27	kPa	298.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
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## Sources

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](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=C687478&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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