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=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
рс	4151.61	kPa	Joback Method
ripol	1356.00		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
tb	427.25 ± 0.50	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/mol×K	657.66	Joback Method	
cpg	212.77	J/mol×K	511.13	Joback Method	
cpg	220.46	J/mol×K	540.44	Joback Method	
cpg	235.00	J/mol×K	599.05	Joback Method	
cpg	241.86	J/mol×K	628.35	Joback Method	
cpg	227.87	J/mol×K	569.74	Joback Method	
cpg	204.80	J/mol×K	481.83	Joback Method	
dvisc	0.0255824	Pa×s	264.09	Joback Method	
dvisc	0.0023843	Paxs	336.67	Joback Method	
dvisc	0.0010292	Pa×s	372.96	Joback Method	
dvisc	0.0001769	Paxs	481.83	Joback Method	
dvisc	0.0005156	Pa×s	409.25	Joback Method	
dvisc	0.0002891	Paxs	445.54	Joback Method	
dvisc	0.0067671	Pa×s	300.38	Joback Method	
pvap	0.56	kPa	308.20	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	0.27	kPa	298.40	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	
рvар	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	0.28	kPa	298.40	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	0.21	kPa	295.20	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	
рvар	0.16	kPa	291.30	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	0.11	kPa	286.20	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	0.08	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

Sources

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

Renewable platform chemicals: Evaluation of thermochemical data of any action with complementary experimental and computational methods: https://www.doi.org/10.1016/j.jct.2018.07.029 https://en.wikipedia.org/wiki/Joback_method

http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formationhf: Enthalpy of formation at standard conditionshfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws:Log10 of Water solubility in mol/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volume

pc: Critical Pressurepvap: Vapor pressure

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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