Propanoic acid, 2-hydroxy-, propyl ester

Other names:	lactic acid, propyl ester
	propyl 2-hydroxypropanoate
	propyl lactate
Inchi:	InChI=1S/C6H12O3/c1-3-4-9-6(8)5(2)7/h5,7H,3-4H2,1-2H3
InchiKey:	ILVGAIQLOCKNQA-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CCCOC(=O)C(C)O
Mol. weight [g/mol]:	132.16
CAS:	616-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-373.54	kJ/mol	Joback Method
hf	-569.48	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	897.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1424.00		NIST Webbook
tb	444.00 ± 3.00	K	NIST Webbook
tc	679.05	K	Joback Method
tf	233.00 ± 3.00	K	NIST Webbook
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.29	J/mol×K	679.05	Joback Method
cpg	254.84	J/mol×K	533.77	Joback Method

cpg	263.60	J/mol×K	562.82	Joback Method
cpg	272.02	J/mol×K	591.88	Joback Method
cpg	280.10	J/mol×K	620.94	Joback Method
cpg	287.86	J/mol×K	649.99	Joback Method
cpg	245.76	J/mol×K	504.71	Joback Method
dvisc	0.0210426	Pa×s	275.36	Joback Method
dvisc	0.0055735	Pa×s	313.59	Joback Method
dvisc	0.0019703	Pa×s	351.81	Joback Method
dvisc	0.0008540	Pa×s	390.03	Joback Method
dvisc	0.0004297	Pa×s	428.26	Joback Method
dvisc	0.0002420	Pa×s	466.49	Joback Method
dvisc	0.0001487	Pa×s	504.71	Joback Method
hvapt	52.10	kJ/mol	388.00	NIST Webbook
pvap	0.14	kPa	299.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.16	kPa	301.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.19	kPa	304.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.26	kPa	308.10	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.12	kPa	298.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.36	kPa	313.60	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.43	kPa	316.00	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.45	kPa	317.00	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.57	kPa	320.00	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.66	kPa	323.00	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.09	kPa	294.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.08	kPa	292.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.07	kPa	290.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.06	kPa	287.80	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.05	kPa	286.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.05	kPa	286.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.04	kPa	283.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.03	kPa	282.10	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.03	kPa	279.90	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.02	kPa	277.70	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.02	kPa	276.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.02	kPa	274.60	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.02	kPa	273.50	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.34	kPa	312.10	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
High-pressure phase behavior of propyl lactate and butyl lactate in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2011.10.010
Renewable platform chemicals:	https://www.doi.org/10.1016/j.jct.2018.07.029
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=C616091&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume