Propanoic acid, 2-hydroxy-, pentyl ester

Other names:	amyl lactate
	lactic acid, pentyl ester
	n-Amyl lactate
	pentyl 2-hydroxypropanoate
	pentyl lactate
Inchi:	InChI=1S/C8H16O3/c1-3-4-5-6-11-8(10)7(2)9/h7,9H,3-6H2,1-2H3
InchiKey:	GXOHBWLPQHTYPF-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCCCOC(=O)C(C)O
Mol. weight [g/mol]:	160.21
CAS:	6382-06-5

Physical Properties

Property code	Value	Unit	Source
gf	-356.70	kJ/mol	Joback Method
hf	-610.76	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.101		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1610.00		NIST Webbook
tb	550.47	K	Joback Method
tc	722.09	K	Joback Method
tf	251.00 ± 2.00	K	NIST Webbook
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.29	J/mol×K	722.09	Joback Method
cpg	344.69	J/mol×K	579.07	Joback Method
cpg	355.26	J/mol×K	607.68	Joback Method
cpg	365.40	J/mol×K	636.28	Joback Method
cpg	375.11	J/mol×K	664.88	Joback Method
cpg	384.41	J/mol×K	693.49	Joback Method
cpg	333.69	J/mol×K	550.47	Joback Method
dvisc	0.0001680	Pa×s	508.38	Joback Method
dvisc	0.0002959	Pa×s	466.28	Joback Method
dvisc	0.0005834	Pa×s	424.19	Joback Method
dvisc	0.0013358	Pa×s	382.09	Joback Method
dvisc	0.0037547	Pa×s	340.00	Joback Method
dvisc	0.0001040	Pa×s	550.47	Joback Method
dvisc	0.0141338	Pa×s	297.90	Joback Method
hvapt	73.90	kJ/mol	378.50	NIST Webbook
pvap	0.07	kPa	315.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.09	kPa	319.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.11	kPa	321.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.06	kPa	313.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.14	kPa	325.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.17	kPa	327.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.19	kPa	329.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.22	kPa	331.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.25	kPa	333.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.28	kPa	335.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.31	kPa	337.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.35	kPa	339.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	
pvap	0.42	kPa	341.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods	

pvap	0.47	kPa	343.20	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.05	kPa	311.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.04	kPa	309.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.04	kPa	307.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.03	kPa	305.30	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

pvap	0.03	kPa	303.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.08	kPa	317.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods
pvap	0.13	kPa	323.40	Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6382065&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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