cis-3-Hexenyllactate

Other names:	Lactic acid cis-3-hexenyl ester
	Propanoic acid, 2-hydroxy-, 3-hexenyl ester, (Z)-
	(Z)-hex-3-enyl lactate
Inchi:	InChI=1S/C9H16O3/c1-3-4-5-6-7-12-9(11)8(2)10/h4-5,8,10H,3,6-7H2,1-2H3/b5-4-
InchiKey:	NNLLMULULOBXBY-PLNGDYQASA-N
Formula:	C9H16O3
SMILES:	CCC=CCCOC(=O)C(C)O
Mol. weight [g/mol]:	172.22
CAS:	61931-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-268.06	kJ/mol	Joback Method
hf	-514.18	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.267		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1187.00		NIST Webbook
ripol	1727.00		NIST Webbook
ripol	1727.00		NIST Webbook
tb	577.51	K	Joback Method
tc	754.42	K	Joback Method
tf	304.09	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.75	J/mol×K	577.51	Joback Method
cpg	372.07	J/mol×K	606.99	Joback Method
cpg	382.88	J/mol×K	636.48	Joback Method

cpg	393.19	J/mol×K	665.96	Joback Method
cpg	403.02	J/mol×K	695.45	Joback Method
cpg	412.39	J/mol×K	724.93	Joback Method
cpg	421.31	J/mol×K	754.42	Joback Method
dvisc	0.0115818	Pa×s	304.09	Joback Method
dvisc	0.0028644	Pa×s	349.66	Joback Method
dvisc	0.0009777	Pa×s	395.23	Joback Method
dvisc	0.0004168	Pa×s	440.80	Joback Method
dvisc	0.0002084	Pa×s	486.37	Joback Method
dvisc	0.0001174	Pa×s	531.94	Joback Method
dvisc	0.0000724	Pa×s	577.51	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C61931815&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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