Linalyl acetate

Other names:	(.+/-.)-Linalyl acetate
	1,5-Dimethyl-1-vinyl-4-hexenyl acetate
	1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate
	1,6-octadien-3-ol, 3,7-dimethyl-, acetate
	3,7-Dimethyl-1,6-octadien-3-ol acetate
	3,7-dimethyl-1,6-octadien-3-yl acetate
	Bergamiol
	Bergamol
	Bergamot mint oil
	Licareol acetate
	Linalol acetate
	Linaloyl acetate
	Lynalyl acetate
	NSC 2138
	Phanteine
	acetic acid linalool ester
	linalool acetate
Inchi:	InChI=1S/C12H20O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h6,8H,1,7,9H2,2-5H3
InchiKey:	UWKAYLJWKGQEPM-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	C=CC(C)(CCC=C(C)C)OC(C)=O
Mol. weight [g/mol]:	196.29
CAS:	115-95-7

Physical Properties

Property code	Value	Unit	Source
gf	-21.41	kJ/mol	Joback Method
hf	-311.70	kJ/mol	Joback Method
hfus	19.82	kJ/mol	Joback Method
hvap	49.53	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.241		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1238.00		NIST Webbook
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ripol	1538.00		NIST Webbook
tb	493.20	K	NIST Webbook
tb	493.15	K	Liquid-Liquid Equilibria of the (Water + Ethanol + Linalyl Acetate) Ternary System at Different Temperatures
tc	740.67	K	Joback Method
tf	278.78	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.02	J/mol×K	644.20	Joback Method
cpg	487.46	J/mol×K	676.36	Joback Method
cpg	500.16	J/mol×K	708.51	Joback Method
cpg	428.80	J/mol×K	547.74	Joback Method
cpg	444.73	J/mol×K	579.89	Joback Method
cpg	459.79	J/mol×K	612.05	Joback Method
cpg	512.14	J/mol×K	740.67	Joback Method

hvapt	62.50	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography
hvapt	57.80	kJ/mol	385.50	NIST Webbook
hvapt	56.80	kJ/mol	410.50	NIST Webbook

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
101.80	298.15	898.64

Reference *https://www.doi.org/10.1016/j.jct.2013.11.026*

Temperature, K	Pressure, kPa	Mass density, kg/m3
298.15	100.00	898.6

Reference *https://www.doi.org/10.1021/acs.jced.8b00939*

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015
Viscosities and densities of systems involved in the deterpenation of essential oils by liquid-liquid extraction: New UNIFAC-VISCO parameters:	https://www.doi.org/10.1016/j.jct.2013.11.026
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115957&Units=SI
Physical Properties of Model and Real Systems Composed of Essential Oils and Hydroalcoholic Solvents at 298.2 K and Atmospheric Pressure:	https://www.doi.org/10.1021/acs.jced.8b00939
Liquid-Liquid Equilibria of the (Water + Ethanol + Linalyl Acetate) Ternary System at Different Temperatures:	https://www.doi.org/10.1021/je101035p
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rhol:	Liquid Density
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

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