

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:	<chem>C=CC(C)(CCC=C(C)C)OC(C)=O</chem>
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	1237.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1239.00		NIST Webbook

rinpol	1239.00	NIST Webbook
rinpol	1239.70	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1253.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1272.00	NIST Webbook

rinpol	1246.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1239.40	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1240.13	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1240.00	NIST Webbook

rinpol	1258.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1239.20	NIST Webbook
rinpol	1242.50	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1253.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1241.00	NIST Webbook

rinpol	1259.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1223.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1259.40	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1240.00	NIST Webbook

rinpol	1257.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1235.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1237.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1232.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1266.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1251.00	NIST Webbook

rinpol	1256.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1263.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1281.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1256.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1281.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1255.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1261.00	NIST Webbook

ripol	1251.00	NIST Webbook
ripol	1555.00	NIST Webbook
ripol	1535.00	NIST Webbook
ripol	1538.00	NIST Webbook
ripol	1551.00	NIST Webbook
ripol	1555.00	NIST Webbook
ripol	1543.00	NIST Webbook
ripol	1560.00	NIST Webbook
ripol	1555.00	NIST Webbook
ripol	1541.00	NIST Webbook
ripol	1525.00	NIST Webbook
ripol	1568.00	NIST Webbook
ripol	1555.00	NIST Webbook
ripol	1559.00	NIST Webbook
ripol	1528.00	NIST Webbook
ripol	1569.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1575.00	NIST Webbook
ripol	1549.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1549.00	NIST Webbook
ripol	1545.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1570.00	NIST Webbook
ripol	1549.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1554.00	NIST Webbook
ripol	1553.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1553.00	NIST Webbook
ripol	1557.00	NIST Webbook
ripol	1550.00	NIST Webbook
ripol	1545.00	NIST Webbook
ripol	1563.00	NIST Webbook
ripol	1556.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1538.00	NIST Webbook
ripol	1552.00	NIST Webbook
ripol	1557.00	NIST Webbook
ripol	1579.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1557.00	NIST Webbook
ripol	1564.00	NIST Webbook

ripol	1555.00	NIST Webbook
ripol	1530.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1552.00	NIST Webbook
ripol	1556.00	NIST Webbook
ripol	1568.00	NIST Webbook
ripol	1568.00	NIST Webbook
ripol	1569.00	NIST Webbook
ripol	1553.00	NIST Webbook
ripol	1553.00	NIST Webbook
ripol	1560.00	NIST Webbook
ripol	1543.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1544.00	NIST Webbook
ripol	1551.00	NIST Webbook
ripol	1571.00	NIST Webbook
ripol	1559.00	NIST Webbook
ripol	1583.00	NIST Webbook
ripol	1569.00	NIST Webbook
ripol	1574.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1555.00	NIST Webbook
ripol	1542.00	NIST Webbook
ripol	1558.00	NIST Webbook
ripol	1554.00	NIST Webbook
ripol	1553.00	NIST Webbook
ripol	1556.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1527.00	NIST Webbook
ripol	1548.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1538.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1537.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1566.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1565.00	NIST Webbook

ripol	1554.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	493.15	K	Liquid-Liquid Equilibria of the (Water + Ethanol + Linalyl Acetate) Ternary System at Different Temperatures
tb	493.20	K	NIST Webbook
tc	740.67	K	Joback Method
tf	278.78	K	Joback Method
vc	0.682	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Viscosities and densities of systems involved in the deterpenation of Essential Oils of Real and Real Systems Composed of Essential Oils and Hydroalcoholic Solvents at 298.2 K and Atmospheric Pressure: Crippen Method:	https://www.doi.org/10.1016/j.jct.2013.11.026
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115957&Units=SI
Liquid-Liquid Equilibria of the (Water + Ethanol + Linalyl Acetate) Ternary System at Different Temperatures:	https://www.doi.org/10.1021/je101035p

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
rho:	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

Latest version available from:

<https://www.cheméo.com/cid/19-704-9/Linalyl-acetate.pdf>

Generated by Cheméo on 2024-04-24 10:02:47.182189239 +0000 UTC m=+16242216.102766555.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.