2,6-Octadienal, 3,7-dimethyl-

Other names:	(2E)-3,7-Dimethyl-2,6-octadienal
	2,6-octadienal, 3,7-dimethyl-, (cis+trans)
	3,7-Dimethyl-1,2,6-octadienal
	3,7-Dimethyl-2,6-octadien-1-al
	3,7-Dimethyl-2,6-octadienal
	3,7-Dimethyl-2,6-octadiene-1-al
	3,7-dimethyl-2,6-octadienal (cis+trans)
	Citral
	Citral (cis and trans)
	Citral acis-3,7-dimethyl-2,6-octadienal
	Citral,c&t
	Lemarome n
	Lemsyn GB
	NCI-C56348
	NSC 6170
	Neral
	Z-3,7-Dimethyl-2,6-octadiene-1-al
	cis,trans-Citral
	cis-Citral
Inchi:	InChI=1S/C10H16O/c1-9(2)5-4-6-10(3)7-8-11/h5,7-8H,4,6H2,1-3H3
InchiKey:	WTEVQBCEXWBHNA-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC(C)=CCCC(C)=CC=O
Mol. weight [g/mol]:	152.23
CAS:	5392-40-5

Physical Properties

Property code	Value	Unit	Source
gf	77.14	kJ/mol	Joback Method
hf	-120.45	kJ/mol	Joback Method
hfus	21.73	kJ/mol	Joback Method
hvap	55.90	kJ/mol	NIST Webbook
log10ws	-2.06		Estimated Solubility Method
log10ws	-2.06		Aqueous Solubility Prediction Method
logp	2.878		Crippen Method

mcvol	144.730	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1242.50		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1240.50		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1240.60		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1240.50		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1216.00		NIST Webbook
ripol	1717.50		NIST Webbook
ripol	1717.50		NIST Webbook
ripol	1720.40		NIST Webbook
ripol	1716.20		NIST Webbook
ripol	1717.50		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1706.00		NIST Webbook
tb	502.20	K	NIST Webbook
tc	675.98	K	Joback Method
tf	206.38	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.25	J/mol×K	644.14	Joback Method
cpg	309.04	J/mol×K	484.94	Joback Method
cpg	322.90	J/mol×K	516.78	Joback Method
cpg	336.01	J/mol×K	548.62	Joback Method
cpg	348.41	J/mol×K	580.46	Joback Method
cpg	360.14	J/mol×K	612.30	Joback Method
cpg	381.76	J/mol×K	675.98	Joback Method

cpl	304.50	J/mol×K	293.00	NIST Webbook
dvisc	0.0008420	Pa×s	353.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0028220	Pa×s	283.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0022250	Pa×s	293.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0021110	Pa×s	298.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure

dvisc	0.0018070	Pa×s	303.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0015020	Pa×s	313.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0012740	Pa×s	323.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
dvisc	0.0010970	Pa×s	333.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure

dvisc	0.0009560	Pa×s	343.15	Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure
rhol	884.84	kg/m3	298.20	Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
101.80	298.15	883.42

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

Sources

Density, Viscosity, and Refractive Index in the Range (283.15 to 353.15) K and Vapor Pressure of r-Pinene, d-Limonene, (()-Linalool, and Citral Over the Pressure Range 1.0 kPa Atmospheric Pressure:	https://www.doi.org/10.1021/je8007414
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5392405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Liquid Equilibria Measurements of Bitter Orange Aroma Compounds Highly Diluted in Boiling Hydro-Alcoholic Solutions at 101.3 kPa:	https://www.doi.org/10.1021/je3004854
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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