Citronellal

Other names:	(.+-.)-citronellal
	.beta.-citronellal
	2,3-Dihydrocitral
	3,7-Dimethyl-6-octenal
	3,7-dimethyl-6-octen-1-al
	6-Octenal, 3,7-dimethyl-
	Citronelal
	Citronella
	Citronellel
	NSC 46106
	Rhodinal
	«beta»-Citronellal
	Â«betaÂ»-Citronellal
Inchi:	InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,8,10H,4,6-7H2,1-3H3
InchiKey:	NEHNMFOYXAPHSD-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CC(C)=CCCC(C)CC=O
Mol. weight [g/mol]:	154.25
CAS:	106-23-0

Physical Properties

Property code	Value	Unit	Source
gf	3.03	kJ/mol	Joback Method
hf	-233.16	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	44.22	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.958		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1161.00		NIST Webbook
rinpol	1122.30		NIST Webbook
rinpol	1153.00		NIST Webbook
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ripol	1495.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1488.00		NIST Webbook
tb	481.00 ± 0.50	K	NIST Webbook
tc	663.60	K	Joback Method
tf	210.42	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.40	J/mol×K	633.07	Joback Method
cpg	326.12	J/mol×K	480.46	Joback Method
cpg	340.49	J/mol×K	510.98	Joback Method
cpg	354.17	J/mol×K	541.51	Joback Method
cpg	367.20	J/mol×K	572.03	Joback Method
cpg	379.60	J/mol×K	602.55	Joback Method
cpg	402.62	J/mol×K	663.60	Joback Method
rhol	856.30	kg/m3	298.20	Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49679e+01
Coeff. B	-4.20573e+03
Coeff. C	-7.46320e+01
Temperature range (K), min.	361.12
Temperature range (K), max.	510.17

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.20	850.03

Sources

Deterpenation of eucalyptus essential oil by liquid + liquid extraction: Phase equilibrium and physical properties for model systems at T = 298.2 K:	https://www.doi.org/10.1016/j.jct.2013.09.044
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106230&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Measurement and Correlation of Citronellal and Methyl Anthranilate Solubilities in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.5b00423
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Physical Behavior of the Phases from the Liquid-Liquid Equilibrium of Citrus Essential Oils Systems at 298.2 K:	https://www.doi.org/10.1021/acs.jced.8b00086
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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