

Citronellol

Other names:	(.+-)-3,7-dimethyl-6-octen-1-ol 2,3-Dihydrogeraniol 2,6-Dimethyl-2-octen-8-ol 3,7-Dimethyl-6-octen-1-ol 3,7-dimethyl-6-octen-1-ol (citronellol) 6-Octen-1-ol, 3,7-dimethyl- Cephrol Elenol NSC 8779 R-(+)-3,7-Dimethyl-6-octen-1-ol R-(+)-«beta»-Citronellol R-(+)-Â«betaÂ»-Citronellol Rhodinol Rodinol dl-Citronellol «beta»-Citronellol Â«betaÂ»-Citronellol
Inchi:	InChI=1S/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h5,10-11H,4,6-8H2,1-3H3
InchiKey:	QMVPMAAFGQKVCJ-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CC(C)=CCCC(C)CO
Mol. weight [g/mol]:	156.27
CAS:	106-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-34.27	kJ/mol	Joback Method
hf	-299.81	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	63.50	kJ/mol	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.751		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1212.51		NIST Webbook
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tb	497.55 ± 0.40	K	NIST Webbook
tb	497.00 ± 1.00	K	NIST Webbook
tc	694.42	K	Joback Method
tf	229.24	K	Joback Method
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.91	J/mol×K	523.98	Joback Method
cpg	376.24	J/mol×K	552.39	Joback Method
cpg	388.99	J/mol×K	580.79	Joback Method
cpg	401.17	J/mol×K	609.20	Joback Method
cpg	412.81	J/mol×K	637.61	Joback Method
cpg	423.93	J/mol×K	666.01	Joback Method
cpg	434.56	J/mol×K	694.42	Joback Method
hsubt	66.10	kJ/mol	308.00	NIST Webbook
hvapt	72.60	kJ/mol	313.00	NIST Webbook
hvapt	65.90	kJ/mol	436.50	NIST Webbook
rhol	855.37	kg/m ³	293.15	(Liquid + liquid) equilibria for (water + 1-propanol or acetone + .beta.-citronellol) at different temperatures

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.62029e+01
Coeff. B	-4.81412e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	353.15
Temperature range (K), max.	521.65

Sources

Ternary (liquid + liquid) equilibria for b-citronellol in aqueous alcohol at different temperature ranges	https://www.doi.org/10.1016/j.jct.2012.04.019
Liquid-liquid equilibria for (water + 1-propanol or acetone + isobutyl alcohol) at different temperatures	https://www.doi.org/10.1016/j.jct.2015.02.013
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=C106229&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor 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

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