1,6-Octadiene, 3,7-dimethyl-

Other names:	(-)-(1S)-cis-pinane
	(-)-(1S,2R,5S)-cis-pinane
	(-)-cis-pinane
	.beta.-citronellene
	2,6-Dimethyl 2,7-octadiene
	3,7-Dimethyl-1,6-octadiene
	3,7-Dimethyl-octa-1,6-diene
	Citronellene
	Dihydromyrcene
	[1S-(1.alpha.,2.beta.,5.alpha.)]-2,6,6-trimethylbicyclo[3.1.1]heptane
	bicyclo[3.1.1]heptane, 2,6,6-trimethyl-,
	pinane, (1S,2R,5S)-(-)-
	pinane, cis-(-)-
	«beta»-Citronellene
	Â«betaÂ»-Citronellene
Inchi:	InChI=1S/C10H18/c1-5-10(4)8-6-7-9(2)3/h5,7,10H,1,6,8H2,2-4H3
InchiKey:	FUDNBFMOXDUIIE-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	C=CC(C)CCC=C(C)C
Mol. weight [g/mol]:	138.25
CAS:	2436-90-0

Physical Properties

Property code	Value	Unit	Source
gf	190.39	kJ/mol	Joback Method
hf	-22.15	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	36.83	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	944.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	947.00		NIST Webbook

rinpol	946.00		NIST Webbook
rinpol	945.00		NIST Webbook
ripol	1049.00		NIST Webbook
ripol	1088.00		NIST Webbook
tb	432.00 ± 3.00	K	NIST Webbook
tc	609.41	K	Joback Method
tf	166.66	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.02	J/mol×K	428.48	Joback Method
cpg	299.14	J/mol×K	458.64	Joback Method
cpg	313.54	J/mol×K	488.79	Joback Method
cpg	327.26	J/mol×K	518.95	Joback Method
cpg	340.32	J/mol×K	549.10	Joback Method
cpg	352.75	J/mol×K	579.26	Joback Method
cpg	364.58	J/mol×K	609.41	Joback Method
rfi	1.44160		293.10	Liquid liquid phase equilibria of the ternary system of water/1,4-dioxane/dihydromyrcene

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53459e+01
Coeff. B	-3.98444e+03
Coeff. C	-6.05790e+01
Temperature range (K), min.	325.18
Temperature range (K), max.	457.66

Sources

Liquid liquid phase equilibria of the ternary system of water/1,4-dioxane/dihydromyrcene:	https://www.doi.org/10.1016/j.fluid.2009.03.017
Isobaric vapor-liquid equilibrium (VLE) for pinane, dihydromyrcene (DHM) and dihydromyrcenol (DHMOH) at 6 kPa:	https://www.doi.org/10.1016/j.fluid.2012.12.035
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Coupled phase-reaction equilibrium for dihydromyrcene hydration system:	https://www.doi.org/10.1016/j.fluid.2016.11.007
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2436900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rfi:	Refractive Index
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