

# «beta»-Pinene

<b>Other names:</b>	(-)-.beta.-pinene (.+/-)-«beta»-Pinene (.+/-)-Â«betaÂ»-Pinene (1S)-(-)-.beta.-pinene (1S,5S)-6,6-dimethyl-2-methylenebicyclo[3.1.1]heptane 2(10)-Pinene 2,2,6-Trimethylbicyclo(3.1.1)hept-2-ene 6,6-Dimethyl-2-methylene-bicyclo[3.1.1]heptane 6,6-dimethyl-2-methylenebicyclo[3.1.1]heptane («beta»-pinene) 6,6-dimethyl-2-methylenebicyclo[3.1.1]heptane (Â«betaÂ»-pinene) Bicyclo[3.1.1] heptane-6,6-dimethyl-2-methyl Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- Bicyclo[3.1.1]heptane-6,6-trimethyl, 2-methylene NSC 21447 Nopinene Nopinene Pinene, «beta» Pinene, Â«betaÂ» Pseudopinene Pseudopinene Terebenthene beta-Pinene pin-2(10)-ene
<b>Inchi:</b>	InChI=1S/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h8-9H,1,4-6H2,2-3H3
<b>InchiKey:</b>	WTARULDDTDQWMU-UHFFFAOYSA-N
<b>Formula:</b>	C10H16
<b>SMILES:</b>	C=C1CCC2CC1C2(C)C
<b>Mol. weight [g/mol]:</b>	136.23
<b>CAS:</b>	127-91-3

## Physical Properties

Property code	Value	Unit	Source
chl	-6214.10 ± 2.90	kJ/mol	NIST Webbook
gf	182.60	kJ/mol	Joback Method
hf	-31.15	kJ/mol	Joback Method
hfus	9.44	kJ/mol	Joback Method

hvap	45.80 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	974.00		NIST Webbook
rinpol	977.62		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	980.30		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1009.00		NIST Webbook
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ripol	1093.00		NIST Webbook
ripol	1100.00		NIST Webbook
tb	440.68	K	Joback Method
tc	648.22	K	Joback Method
tf	211.60	K	Solid-Liquid Equilibria in Binary Mixtures of 1,8-Cineole with p-Cymene, beta-Pinene, and Camphene
tf	211.61 ± 0.10	K	NIST Webbook
vc	0.482	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.71	J/mol×K	440.68	Joback Method
cpg	291.03	J/mol×K	475.27	Joback Method
cpg	308.01	J/mol×K	509.86	Joback Method
cpg	323.77	J/mol×K	544.45	Joback Method
cpg	338.45	J/mol×K	579.04	Joback Method
cpg	352.17	J/mol×K	613.63	Joback Method
cpg	365.06	J/mol×K	648.22	Joback Method
hvapt	46.00	kJ/mol	364.50	NIST Webbook
hvapt	41.60	kJ/mol	401.50	NIST Webbook
hvapt	43.47	kJ/mol	288.00	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35512e+01
Coeff. B	-3.35712e+03
Coeff. C	-6.32450e+01
Temperature range (K), min.	316.35
Temperature range (K), max.	470.67

## Datasets

### Mass density, kg/m<sup>3</sup>

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m <sup>3</sup> - Liquid
283.15	20000.00	891.3
283.15	25000.00	894.2
283.15	30000.00	897.0
283.15	35000.00	899.9
283.15	40000.00	902.6
298.15	20000.00	880.2
298.15	25000.00	883.3
298.15	30000.00	886.3
298.15	35000.00	889.3
298.15	40000.00	892.2
313.15	20000.00	869.3
313.15	25000.00	872.6
313.15	30000.00	875.7
313.15	35000.00	878.8
313.15	40000.00	882.0
328.15	20000.00	858.2
328.15	25000.00	861.7
328.15	30000.00	865.2
328.15	35000.00	868.7
328.15	40000.00	872.2

343.15	20000.00	847.7
343.15	25000.00	851.4
343.15	30000.00	855.0
343.15	35000.00	858.6
343.15	40000.00	862.1
358.15	20000.00	837.0
358.15	25000.00	840.9
358.15	30000.00	844.8
358.15	35000.00	848.7
358.15	40000.00	852.6

Reference

<https://www.doi.org/10.1016/j.jct.2011.12.013>

## Sources

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Crippen Method:

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## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>h<sub>vapt</sub>:</b>	Enthalpy of vaporization at a given temperature
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rho<sub>l</sub>:</b>	Liquid Density

<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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