

Limonene

Other names:

(R/ S)-limonene
(+)-(4R)-limonene
(+)-limonene
(-)-.beta.-pinene
(.+/-.)-Dipentene
(.+/-.)-Limonene
(.+/-.)-«alpha»-Limonene
(1S)-(-)-.beta.-pinene
(1S,5S)-6,6-dimethyl-2-methylenebicyclo[3.1.1]heptane
(R)-(+)-Limonene
(R)-Limonene
(±)-limonene
1,8(9)-p-Menthadiene
1,8-p-Menthadiene
1-Methyl-4-(1-methylethenyl)cyclohexene
1-Methyl-4-isopropenyl-1-cyclohexene
1-Methyl-4-isopropenylcyclohexene
1-methyl-4-(prop-1-en-2-yl)cyclohex-1-ene
1-methyl-4-isopropenylcyclohex-1-ene
1-methyl-4-isopropenylcyclohex-1-ene (limonene)
4-Isopropenyl-1-methyl-1-cyclohexene
4-Isopropenyl-1-methylcyclohexene
Achilles dipentene
Acintene DP
Acintene DP dipentene
Cajeputen
Cajeputene
Cinen
Cinene
Cyclohexene, 1-methyl-4-(1-methylethenyl)-
Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (.+/-.)-
Cyclohexene, 1-methyl-4-(1-methylethynyl)
D-Limonene
DL-Limonene
Di-p-mentha-1,8-diene
Dipanol
Dipenten
Dipentene
Dipentene limonene
Eulimen

Flavor orange
Goldflush II
Inactive limonene
Kautschin
Limonen
Limonene [4R-(+), 4S-(-)]
Limonene+
NSC 21446
Nesol
Orange flavor
PC 560
UN 2052
Unitene
dipentene (p-Mentha-1,8-diene)
p-Mentha-1,8(9)-diene
p-Mentha-1,8-diene
p-Mentha-1,8-diene, dl-
«alpha»-Limonene
«delta»-1,8-Terpodiene

Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3
InchiKey: XMGQYMWWDOXHJM-UHFFFAOYSA-N
Formula: C10H16
SMILES: C=C(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 136.23
CAS: 7705-14-8

Physical Properties

Property code	Value	Unit	Source
chl	-6171.00 ± 2.10	kJ/mol	NIST Webbook
gf	157.39	kJ/mol	Joback Method
hf	-33.46	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	38.65	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	449.15 ± 1.00	K	NIST Webbook
tb	451.20	K	NIST Webbook
tc	657.16	K	Joback Method

tf	207.40	K	Joback Method
vc	0.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.80	J/mol×K	448.45	Joback Method
cpg	287.42	J/mol×K	483.23	Joback Method
cpg	304.13	J/mol×K	518.02	Joback Method
cpg	319.94	J/mol×K	552.80	Joback Method
cpg	334.90	J/mol×K	587.59	Joback Method
cpg	349.03	J/mol×K	622.37	Joback Method
cpg	362.36	J/mol×K	657.16	Joback Method
rhoI	866.84	kg/m ³	298.15	Ternary and quaternary (liquid + liquid) equilibria for (water + ethanol + a-pinene, +b-pinene, or +limonene) and (water + ethanol + a-pinene + limonene) at the temperature 298.15 K

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7705148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Ternary and quaternary (liquid + liquid) equilibria for (water + ethanol + a-pinene, +b-pinene, or +limonene) and (water + ethanol + a-pinene + limonene) at the temperature 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.10.018
Joback Method	https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion

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
rho:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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