

Limonene

Other names: Cyclohexene, 1-methyl-4-(1-methylethenyl)-
p-Mentha-1,8-diene
«alpha»-Limonene
Cajeputen
Cajeputene
Cinen
Cinene
Dipenten
Dipentene
Eulimen
Kautschin
Limonen
Nesol
p-Mentha-1,8(9)-diene
«delta»-1,8-Terpodiene
p-Mentha-1,8-diene, dl-
Acintene DP dipentene
Di-p-mentha-1,8-diene
DL-Limonene
Inactive limonene
1-Methyl-4-isopropenyl-1-cyclohexene
1,8(9)-p-Menthadiene
4-Isopropenyl-1-methyl-1-cyclohexene
Acintene DP
Dipanol
UN 2052
Unitene
4-Isopropenyl-1-methylcyclohexene
1,8-p-Menthadiene
1-Methyl-4-(1-methylethenyl)cyclohexene
1-Methyl-4-isopropenylcyclohexene
(.+/-)-Limonene
Achilles dipentene
1-methyl-4-isopropenylcyclohex-1-ene
1-methyl-4-(prop-1-en-2-yl)cyclohex-1-ene
Cyclohexene, 1-methyl-4-(1-methylethynyl)
Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (.+/-)-
(.+/-)-Dipentene
(.+/-)-«alpha»-Limonene
Flavor orange

Goldflush II
 NSC 21446
 Orange flavor
 PC 560
 Dipentene limonene
 D-Limonene
 (+)-limonene
 (+)-(4R)-limonene
 (R/ S)-limonene
 (R)-(+)-Limonene
 (R)-Limonene
 (±)-limonene
 Limonene [4R-(+), 4S-(-)]
 1-methyl-4-isopropenylcyclohex-1-ene (limonene)
 dipentene (p-Mentha-1,8-diene)
 Limonene+

Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3
InchiKey: XMGQYMWWD0XHJM-UHFFFAOYSA-N
Formula: C10H16
SMILES: C=C(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 136.23
CAS: 138-86-3

Physical Properties

Property code	Value	Unit	Source
chl	-6128.30	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
ie	8.30	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	1020.30		NIST Webbook
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ripol	1183.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1200.00		NIST Webbook
tb	454.00 ± 4.00	K	NIST Webbook
tb	448.20	K	NIST Webbook
tb	448.00 ± 4.00	K	NIST Webbook
tb	450.75 ± 0.35	K	NIST Webbook
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tb	450.00 ± 4.00	K	NIST Webbook
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tb	450.00 ± 5.00	K	NIST Webbook
tb	452.00 ± 4.00	K	NIST Webbook
tb	454.00 ± 4.00	K	NIST Webbook
tb	451.00 ± 4.00	K	NIST Webbook
tc	657.16	K	Joback Method
tf	177.65 ± 0.30	K	NIST Webbook
tf	184.12 ± 0.10	K	NIST Webbook
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.90	J/mol×K	587.59	Joback Method
cpg	349.03	J/mol×K	622.37	Joback Method
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	362.36	J/mol×K	657.16	Joback Method
cpl	249.40	J/mol×K	293.30	NIST Webbook
cpl	249.40	J/mol×K	293.40	NIST Webbook
hvapt	39.40	kJ/mol	379.00	NIST Webbook
hvapt	45.90	kJ/mol	367.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C138863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
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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