D-Limonene

Other names:
(+)-(4R)-Limonene
(+)-(R)-Limonene
(+)-Dipentene
(+)-Limonene
(+)-p-Mentha-1,8-diene
(-)-(S)-limonene
(-)-.alpha.-limonene
(-)-limonene
(4R)-(+)-Limonene
(4R)-Limonene
(R)-(+)-Limonene
(R)-(+)-p-Mentha-1,8-diene
(R)-1-methyl-4-(1-methylethenyl)cyclohexene
(R)-4-Isopropenyl-1-methyl-1-cyclohexene
(R)-Limonene
(R)-p-Mentha-1,8-diene
(S)-(-)-limonene
(S)-1-methyl-4-(1-methylethenyl)cyclohexene
(S)-4-isopropenyl-1-methyl-1-cyclohexene
(S)-limonene
.beta.-limonene
4-Isopropenyl-1-methyl-1-cyclohexene-, (R)-
Biogenic SE 374
Carvene
Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (4R)-
Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)-
D-(+)-Limonene
Dextro-limonene
EC 7
Glidesafe
Glidsafe
L-limonene
Limonene, (+)-
Limonene, (D)-
Refchole
cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-,
p-Mentha-1,8-diene, (R)-(+)-
p-mentha-1,8-diene, (S)-(-)-

Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3/t10-/m1/s1

InchiKey: XMGQYMWWDOXHJM-SNVBAGLBSA-N

Formula: C10H16
SMILES: C=C(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 136.23
CAS: 5989-27-5

Physical Properties

Property code	Value	Unit	Source
chl	-6167.20 ± 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	49.60	kJ/mol	NIST Webbook
hvap	48.90 ± 0.10	kJ/mol	NIST Webbook
hvap	49.50	kJ/mol	NIST Webbook
hvap	49.60	kJ/mol	NIST Webbook
hvap	49.90	kJ/mol	NIST Webbook
log10ws	-4.26		Estimated Solubility Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	450.34	K	Measurement and Correlation of Vapor-Liquid Equilibrium Data for ss-Pinene + p-Cymene + (S)-(-)-Limonene at Atmospheric Pressure
tc	657.16	K	Joback Method
tf	198.65 ± 0.15	K	NIST Webbook
vc	0.496	m3/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
hfust	11.38	kJ/mol	199.20	NIST Webbook
hvapt	46.10 ± 0.20	kJ/mol	417.00	NIST Webbook
hvapt	43.50 ± 0.20	kJ/mol	417.00	NIST Webbook
hvapt	40.90 ± 0.30	kJ/mol	417.00	NIST Webbook
hvapt	37.90 ± 0.60	kJ/mol	417.00	NIST Webbook
hvapt	49.20	kJ/mol	342.00	NIST Webbook
hvapt	44.50	kJ/mol	367.50	NIST Webbook
hvapt	47.70	kJ/mol	305.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42584e+01
Coeff. B	-3.89401e+03
Coeff. C	-4.57090e+01
Temperature range (K), min.	324.43
Temperature range (K), max.	480.94

Sources

Measurement and correlation of (vapor + liquid) equilibrium data for (alpha-pinene + p-cymene + (S)-(-)-limonene) ternary system at atmospheric pressure:	https://www.doi.org/10.1016/j.jct.2012.10.017
Measurement and Correlation of Vapor-Liquid Equilibrium Data for (alpha-Pinene + p-Cymene + (S)-(-)-Limonene at Atmospheric Pressure:	https://www.doi.org/10.1021/je101151f
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5989275&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/ci990307l

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
hfust:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume