REFERENCE 9

2. IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

Limonene is a colourless liquid at room temperature. The structural formula for limonene is given below. The chemical exists as two optical isomers, *d*- and *l*-limonene, and the racemic mixture dipentene. The purity of commercial *d*-limonene is about 90–96%.

Physical and chemical data on limonene presented in Table 1 were taken from Karlberg & Lindell (1993), unless otherwise stated. Impurities are mainly other monoterpenes, such as myrcene (7-methyl-3-methylene-1,6-octadiene), alpha-pinene (2,6,6-trimethyl-bicyclo[3.1.1]hept-2-ene), alpha-pinene (6,6-dimethyl-2-methylene-bicyclo[3.1.1]heptane), sabinene (2-methyl-5-(1-methylethyl)-bicyclo[3.1.0]hexan-2-ol), and Gamma3-carene ((1S-cis)-3,7,7-trimethyl-bicyclo[4.1.0]hept-2-ene). The vapour pressure of limonene is high and its solubility in water is low, giving a high value of the Henry's law constant, which predicts a high rate of vaporization of limonene.

Table 1: Physical/chemical properties of limonene.[a]

	d-Limonene	l-Limonene	Dipentene
CAS no.	5989-27-5	5989-54-8	138-86-3
Chemical name	(R)-1-methyl-4-(1-methylethenyl) cyclohexene	(S)-1-methyl-4-(1-methylethenyl) cyclohexene	1-methyl-4-(1-methylethenyl) cyclohexene
Empirical formula	$C_{10}H_{16}$	$C_{10}H_{16}$	$C_{10}H_{16}$
Molecular weight	136.23	136.23	136.23
Melting point (°C)	-74.35	-74.35	-95.9
Boiling point (°C)	175.5–176.0	175.5–176.0	175.5–176.0
Density (g/cm^3 at 20°C)	0.8411	0.8422	0.8402
Vapour pressure (Pa at 20°C)	190	190	190
Water solubility (mg/litre at 25°C)	13.8[b]	-	-
Henry's law constant (kPa m^3/mol at 25°C)	34.8[c]	-	-
Log K_{ow}	4.23[d]	-	4.83[e] (limonene)

[a] Conversion factors: 1 ppm = 5.56 mg/m^3; 1 mg/m^3 = 0.177 ppm.
[b] Massaldi & King, 1973; Assessment Tool for the Evaluation of Risk (ASTER) database, Environmental Research Laboratory, US Environmental Protection Agency, Duluth, MN, 1991.
[c] Calculated value (ENVIROFATE database, Office of Toxic Substances, US Environmental Protection Agency, and Syracuse Research Corporation (SRC), New York, NY, 1999).
[d] Calculated value (US EPA, 1990a, 1994).
[e] Calculated value (US EPA, 1994; Log Octanol-Water Partition Coefficient Program (LOGKOW), Syracuse Research Corporation (SRC), New York, NY).