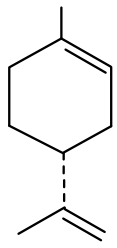
>>**Entry Name: Limonene**

ENTRY UNDER REVIEW

Synonym(s): 1-Methyl-4-(1-methylethenyl)cyclohexene, 9Cl. 4-Isopropenyl-1-methylcyclohexene. *p*-Mentha-1,8-diene. Citrene. Hesperidene. Diisoprene. Terpilene. Kautschine. Cinene. Cynene. Cajeputene. Isoterebentine. Carvene. FEMA 2633



(*R*)-*form*

CAS Registry Number: 138-86-3
Related CAS Registry Numbers(s): 6876-12-6 9003-73-0

Molecular Formula: $C_{10}H_{16}$
Molecular Weight: 136.236
Accurate Mass: 136.1252
Percentage Composition: C 88.16%; H 11.84%
Source/Synthesis: Found in over 300 essential oils, the (*R*)-form is the most widespread, followed by the racemate and then the (*S*)-form
Use/Importance: The most important and widespread terpene known. Extensively used in the perfumery and flavour industries and in manuf. of polymers and adhesives

Aldrich: 33411-1
Fluka: 42560
Rare Chemicals Library: S57073-7

>>**Variant:** (*R*)-form

CAS Registry Number: 5989-27-5

Molecular Formula: $C_{10}H_{16}$
Molecular Weight: 136.236
Accurate Mass: 136.1252
Percentage Composition: C 88.16%; H 11.84%
Biological Source: Major constit. of oil of orange rind, dill oil, oil of cumin, neroli, bergamot, caraway, lemon balm and lemon (*Citrus, Anethum, Juniperus, Peucedanum* spp.) Obt. comly. from orange oil on a large scale (ca. 50000 T/a)
Use/Importance: Important chiral starting material for org. synth. Shows insecticidal props. Flavouring agent. Active principle of lemon balm extract, used for its sedative and antibacterial props.
Physical Description: Oil, with lemon like odour
Boiling Point: Bp_{20} 71°
Optical Rotation: $[\alpha]_D^{20}$+126.8
Hazard & Toxicity: LD_{50} (rat, orl) 4400 mg/kg. Exp. reprod. and teratogenic effects (large doses)

Aldrich: 18316-4
Fluka: 62122
Sigma: L2129
Supelco: S48-2633

>>**Variant:** (*S*)-form

CAS Registry Number: 5989-54-8

Molecular Formula: $C_{10}H_{16}$
Molecular Weight: 136.236
Accurate Mass: 136.1252
Percentage Composition: C 88.16%; H 11.84%
Biological Source: Constit. of pine needle oil. Also present in ginger, nutmeg, pepper, mace, coriander and other herbs and spices
Physical Description: Oil
Boiling Point: Bp 177.6-177.8°
Optical Rotation: $[\alpha]_D$ –122.6
Solubility: BERDY SOL: Sol. MeOH, hexane; poorly sol. H_2O
Hazard & Toxicity: Skin irritant

Aldrich: W50450-5
Fluka: 62128
Supelco: 48-5045