



Guide to Terpene Chemical Properties



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Terpenes are the common term for a large group of compounds that contribute to the flavor and smell of botanical products. Isoprene or 2-methyl-1,3-butadiene (see Figure 1) and its polymers are the main base of natural rubber and the structural base for terpenes and terpenoids, even though isoprene itself is not part of the reactions which produce terpenes.

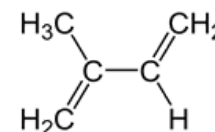


Figure 1. Isoprene Unit

In biological processes, there are essential and non-essential terpenes. Essential terpenes are usually terpenes C15 and higher that are required by the plant, insect or algae to support life and growth. The lower weight terpenes (some C15 and below) are non-essential terpenes that assist in other biological processes or contribute to the defense and functioning of the organism but are not critical to survival.

Terpenes are classified based on the number of isoprene units they contain. Hemiterpenes have 5 carbons; monoterpenes have 10 carbons, sesquiterpenes have 15 carbons, etc. (see Table 1). The classification is based on the C5 rule which is the isoprene synthesis route that organisms employ for the production of terpenes.

Table 1. Terpene Groups

Terpene Group	# Isoprene Units	# Carbons
Hemiterpenes	1	5
Monoterpenes	2	10
Sesquiterpenes	3	15
Diterpenes	4	20
Sesterpenes	5	25
Triterpenes	6	30
Sesquarterpenes	7	35
Tetraterpenes	8	40

Monoterpenes are lower molecular weight terpenes and can volatilize quickly during processing involving heat and decarboxylation. Sesquiterpenes are larger molecular weight terpenes and volatilize at higher temperatures and remain after many processing steps.

The diversity of the terpenes and terpenoids are recognized by the range of scents and flavors they produce from the pine scent of Pinene (the most widely encountered terpene in nature) to the lavender and mint notes associated with Linalool. The flavor and aroma of hops are critical to beer, especially Myrcene, beta-Pinene, beta-Caryophyllene, and alpha-Humulene. Looking for a kit containing all of the terpenes? Our CAN-TERP-KIT contain all 42 terpenes listed below.

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											Solubility (µg/mL @ 20 °C)		
Compound	CAS #	MW	Class	Molecular Formula	BP (°C @ 1 atm)	MP (°C @ 1 atm)	Density (g/cm ³ @ 20°C)	RI (@ 20 °C)	Color	Form	Water	Alcohol	Ether
(-)-alpha-Bisabolol	23089-26-1	222.37	Monocyclic sesquiterpenoid	C ₁₅ H ₂₆ O	290	59.8	0.92	1.492 - 1.498	Clear to Yellow	Liquid	1.68	Miscible	N/D
(+)-Borneol	464-43-7	154.25	Bicyclic Monoterpenoid	C ₁₀ H ₁₈ O	212	202	1.1	N/D	White	Solid	738	Miscible	Miscible
(-)-Borneol	464-45-9	154.25	Bicyclic Monoterpenoid	C ₁₀ H ₁₈ O	210	202	1.1	N/D	White	Solid	738	Miscible	Miscible
Camphene	79-92-5	136.23	Bicyclic Monoterpene	C ₁₀ H ₁₆	160	51.2	0.85	1.4570	White	Waxy Solid	4.6	Slightly Soluble	Miscible
DL-Camphor (mixture of isomers)	76-22-2	152.23	Bicyclic Monoterpenoid	C ₁₀ H ₁₆ O	209	179	0.992	1.5462	Colorless to White	Crystalline Powder	1.2	Miscible	Miscible
D-Camphor	464-49-3	152.23	Bicyclic Monoterpenoid	C ₁₀ H ₁₆ O	205.7	180	0.992	1.5462	Colorless to White	Crystals	1.2	Miscible	Miscible
L-Camphor	464-48-2	152.23	Bicyclic Monoterpenoid	C ₁₀ H ₁₆ O	204	179	0.992	1.5462	Colorless to White	Crystals	1.2	Miscible	Miscible
(1S)-(+)-3-Carene	498-15-7	136.23	Bicyclic Monoterpene	C ₁₀ H ₁₆	170	46	0.854 - 0.8840	1.4710 - 1.4760	Colorless to Light Yellow	Liquid	<1	Slightly Soluble	Miscible
trans-Caryophyllene	87-44-5	204.35	Bicyclic Sesquiterpene	C ₁₅ H ₂₄	262 - 264	<25	0.9075	1.499	Pale yellow	Oily Liquid	<1	N/D	N/D
(-)-Caryophyllene Oxide	1139-30-6	220.36	Bicyclic Sesquiterpenoid	C ₁₅ H ₂₄ O	267	62.5	0.964	1.4956	White to Off-White	Solid	2.21	Miscible	N/D
alpha-Cedrene	469-61-4	204.35	Polycyclic sesquiterpene	C ₁₅ H ₂₄	262.5	N/D	0.932	1.498	Colorless	Oily Liquid	<1	Miscible	N/D
(+)-Cedrol	77-53-2	222.37	Sesquiterpenoid	C ₁₅ H ₂₆ O	286	86	1.01	N/A	White to Yellow	Solid	11.3	Miscible	N/D
Eucalyptol	470-82-6	154.25	Bicyclic Monoterpenoid	C ₁₀ H ₁₈ O	176.4	1.5	0.921 - 0.923	1.4586	Colorless	Liquid	<1	Miscible	Miscible
Farnesene (mixture of isomers)	502-61-4	204.35	Sesquiterpene	C ₁₅ H ₂₄	95 - 125	<25	0.813	1.490 - 1.500	Colorless to Light Green	Liquid	<1	N/D	Miscible
L-Fenchone	7787-20-4	152.23	Bicyclic Monoterpene	C ₁₀ H ₁₆ O	193	N/D	0.945	1.46	Colorless	Liquid	73.1	Miscible	N/D
alpha-Fenchol	2217-02-9	154.25	Bicyclic Monoterpenoid	C ₁₀ H ₁₈ O	201 - 202	45.75	0.942	N/D	Colorless to Light Yellow	Crystals	<1	Miscible	Miscible
(+)-Fenchone	4695-62-9	152.23	Bicyclic Monoterpene	C ₁₀ H ₁₆ O	193.5	6.1	0.948	1.461 - 1.465	Colorless	Oily Liquid	73.14	Miscible	N/D
Geranyl Acetate	105-87-3	196.29	Monoterpenoid	C ₁₂ H ₂₀ O ₂	238.3	<25	0.9174	1.4624	Colorless	Liquid	6.8	Miscible	Miscible
Geraniol	106-24-1	154.25	Monoterpenoid	C ₁₀ H ₁₈ O	227.5	-15	0.8894	1.4710 - 1.4780	Colorless to Yellow	Oily Liquid	100	Miscible	Miscible
Guaiol	489-86-1	222.37	Bicyclic Sesquiterpenoid	C ₁₅ H ₂₆ O	309	40-50	0.965 - 0.975	1.5020 - 1.5070	White to Amber	Crystals or Semisolid	3.61	Miscible	Miscible
alpha-Humulene	6753-98-6	204.35	Monocyclic sesquiterpene	C ₁₅ H ₂₄	167	<25	0.889	1.5	Pale Yellow to Green	Liquid	<1	Miscible	N/D
Isoborneol	124-76-5	154.25	Bicyclic monoterpenoid	C ₁₀ H ₁₈ O	212	202	1.1	1.502	White	Crystalline Solid	738	Miscible	Miscible
(-)-Isopulegol	89-79-2	154.25	Monocyclic monoterpenoid	C ₁₀ H ₁₈ O	218	78	0.904 - 0.913	1.468 - 1.477	White to Yellow	Solid	308.6	Miscible	N/D

* Spex CertiPrep's data shows minimum solubility @ 1,000 µg/mL

** Minimum solubility based on similar cited solvents

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											Solubility (µg/mL @ 20 °C)		
Compound	CAS #	MW	Class	Molecular Formula	BP (°C @ 1 atm)	MP (°C @ 1 atm)	Density (g/cm ³ @ 20°C)	RI (@ 20 °C)	Color	Form	Water	Alcohol	Ether
D-Limonene	5989-27-5	136.23	Monocyclic monoterpene	C ₁₀ H ₁₆	178	-86	0.8411	1.473	Colorless	Oily Liquid	13.8	Miscible	Miscible
Linalool	78-70-6	154.25	Monoterpenoid	C ₁₀ H ₁₈ O	198	<25	0.865	1.4627	Colorless	Liquid	1590	Miscible	Miscible
DL-Menthol	89-78-1	156.26	Monocyclic monoterpenoid	C ₁₀ H ₂₀ O	212	41 - 43	0.89	1.458	White	Crystalline Solid	456	Miscible	Miscible
beta-Myrcene	123-35-3	136.23	Acyclic monoterpene	C ₁₀ H ₁₆	167	-10	0.7601	1.4709	Colorless to Light Yellow	Liquid	5.6	Miscible	N/D
Nerol	106-25-2	154.25	Monoterpenoid	C ₁₀ H ₁₈ O	225	<-15	0.8813	1.4746	Colorless	Liquid	531	Miscible	Miscible
cis-Nerolidol	3790-78-1	222.37	Sesquiterpenoid	C ₁₅ H ₂₆ O	275	-75	0.872 (mix)	1.478 - 1.483 (mix)	Colorless to Light Yellow	Oily Liquid	14.1	Miscible	N/D
trans-Nerolidol	40716-66-3	222.37	Sesquiterpenoid	C ₁₅ H ₂₆ O	275	N/D	0.87	1.48	Colorless to Yellow	Oily Liquid	1.5	Miscible	N/D
beta-Ocimene (mixture of Isomers)	13877-91-3	136.23	Monoterpene	C ₁₀ H ₁₆	65 - 66	N/D	0.818	1.485	Colorless	Liquid	2	N/D	N/D
alpha-Phellandrene	99-83-2	136.23	Monocyclic monoterpene	C ₁₀ H ₁₆	172	N/D	0.841	1.4732	Colorless	Oily Liquid	<1	Miscible	Miscible
alpha-Pinene	80-56-8	136.23	Bicyclic Monoterpene	C ₁₀ H ₁₆	156	-60	0.858	1.4632	Colorless	Liquid	2.49	Miscible	Miscible
beta-Pinene	127-91-3	136.23	Bicyclic Monoterpene	C ₁₀ H ₁₆	166	-61.5	0.86	1.4768	Colorless	Liquid	4.89	Miscible	Miscible
(+)-Pulegone	89-82-7	152.23	Monocyclic monoterpene	C ₁₀ H ₁₆ O	224	<25	0.9323	1.4894	Colorless to Yellow	Oily Liquid	276	Miscible	Miscible
Sabinene	3387-41-5	136.23	Monocyclic monoterpenoid	C ₁₀ H ₁₆	164	N/D	0.842	N/D	Colorless to Light Yellow	Liquid	2.5	Miscible	N/D
Sabinene Hydrate	546-79-2	154.25	Monocyclic monoterpenoid hydrate	C ₁₀ H ₁₈ O	201	60	N/D	N/D	White	Crystals	440	Miscible	N/D
alpha-Terpinene	99-86-5	136.23	Monocyclic monoterpene	C ₁₀ H ₁₆	175	-31	N/D	1.475	Colorless to Light Yellow	Liquid	5.92	Miscible	N/D
gamma-Terpinene	99-85-4	136.23	Monocyclic monoterpene	C ₁₀ H ₁₆	183	-10	N/D	1.475	Colorless to Light Yellow	Liquid	8.68	Miscible	N/D
Terpineol (mixture of Isomers)	8000-41-7	154.25	Monocyclic monoterpenoid	C ₁₀ H ₁₈ O	219	37	0.935	1.4831	Colorless to White	Crystals	710	Miscible	Miscible
Terpinolene	586-62-9	136.23	Monocyclic monoterpene	C ₁₀ H ₁₆	186	<25	0.861	1.4883	White to Light amber	Liquid	9.5	Miscible	Miscible
Valencene	4630-07-3	204.35	Bicyclic Sesquiterpene	C ₁₅ H ₂₄	274	N/D	0.92	1.504	Colorless to Light Yellow	Liquid	<1	Miscible	N/D

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** Minimum solubility based on similar cited solvents