

Fresh Marine Notes

1-Methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde and its dihydro derivatives

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1-Methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde and 1-methyl-4-(4-methylpentyl)cyclohex-3-ene-1-carbaldehyde are two chemically and olfactively related cyclic aldehydes. 1-Methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde (Precyclemonone B)^a is a colorless to pale yellow liquid with an aldehydic, fresh, powerful marine, floral odor (see **F-1**). Reminiscent of lily of the valley leaves, it is a very intensive and substantive material, with incense and sea breeze nuances.*

The commercial material is practically a mixture of two isomers—1-methyl-4-(4-methyl-3-pentenyl)-3-cyclohexene-1-carbaldehyde and 1-methyl-3-(4-methyl-3-pentenyl)-3-cyclohexene-1-carbaldehyde—which due to its clean, tenacious ozone note and aldehydic warmth and diffusion, can be used as a booster for fragrances requiring fresh outdoor effect (see **F-2**). For instance, consider the “clean” trend of the mid 1990s that was an endless variation on three main themes: marine, watery and ozonic notes. Here, different molecules and fragrance structures were used to express the primary idea of water—salty and cold, fresh and somewhat sweet and airy. The marine note is correspondent to the sea shore and the salty and iodine note of algae, and is well represented in 1-methyl-4-(4-methyl-3-pentenyl)-cyclohex-3-ene-1-carbaldehyde. The recommended use level for this mixture of isomers is 10% maximum, and its substantivity lasts for more than two days. The ingredient is generally applied in alcoholic lotions, deodorant sticks, fabric softener and shampoos.

Furthermore, as this aroma ingredient can be derived from 1-methyl-4-(4-methyl-3-pentenyl)-3-cyclohexene-1-carbaldehyde and 1-methyl-3-(4-methyl-3-pentenyl)-3-cyclohexene-1-carbaldehyde, it is also a mixture of isomers 1-methyl-4-(4-methylpentyl)-cyclohex-3-enecarbaldehyde and 1-methyl-3-(4-methylpentyl)-cyclohex-3-enecarbaldehyde (see **F-3**).

^a Precyclemonone B is a trademark of IFF.

*Most of the information on organoleptic properties and uses are taken from: PMP 96, *Database of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, Netherlands. Additional organoleptic information and uses are cited from suppliers specification sheets, e.g. IFF and Givaudan.

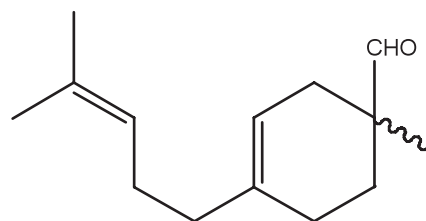


1-Methyl-4-(4-methylpentyl)cyclohex-3-ene-1-carbaldehyde (Vernaldehyde)^b is a colorless to pale yellow liquid with a fresh, green, mountain air character, and blends well with aldehydic citrus and woody notes (see **F-4**). The product adds originality to a fragrance and imparts a natural aura. The unique freshness and diffusion of this ingredient is vividly demonstrated when applied to floral blends such as lily of the valley and lilac. 1-Methyl-4-(4-methylpentyl)cyclohex-3-ene-1-carbaldehyde can stay on a blotter for one day and has a recommended use level of up to 5%. It is most suitable for fine fragrances, beauty care products, soaps, laundry care and household applications.

^b Vernaldehyde is a registered trademark of Givaudan.

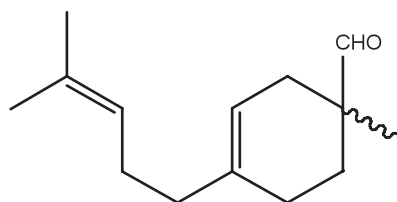
1-Methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde

F-1

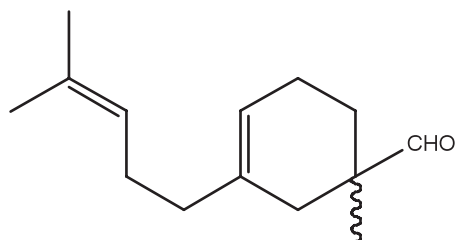


Two isomers of 1-methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde

F-2



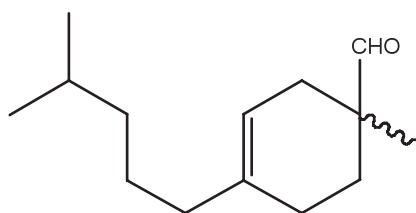
1-Methyl-4-(4-methyl-3-pentenyl)-3-cyclohexene-1-carbaldehyde



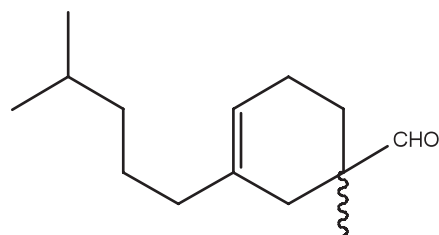
1-Methyl-3-(4-methyl-3-pentenyl)-3-cyclohexene-1-carbaldehyde

Two isomers of 1-methyl-4-(4-methylpentyl)cyclohex-3-ene-1-carbaldehyde

F-3



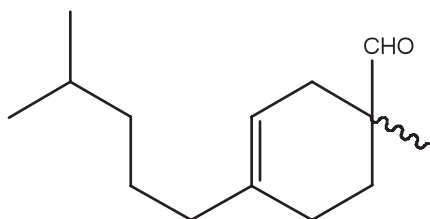
1-Methyl-4-(4-methylpentyl)-cyclohex-3-enecarbaldehyde



1-Methyl-3-(4-methylpentyl)-cyclohex-3-enecarbaldehyde

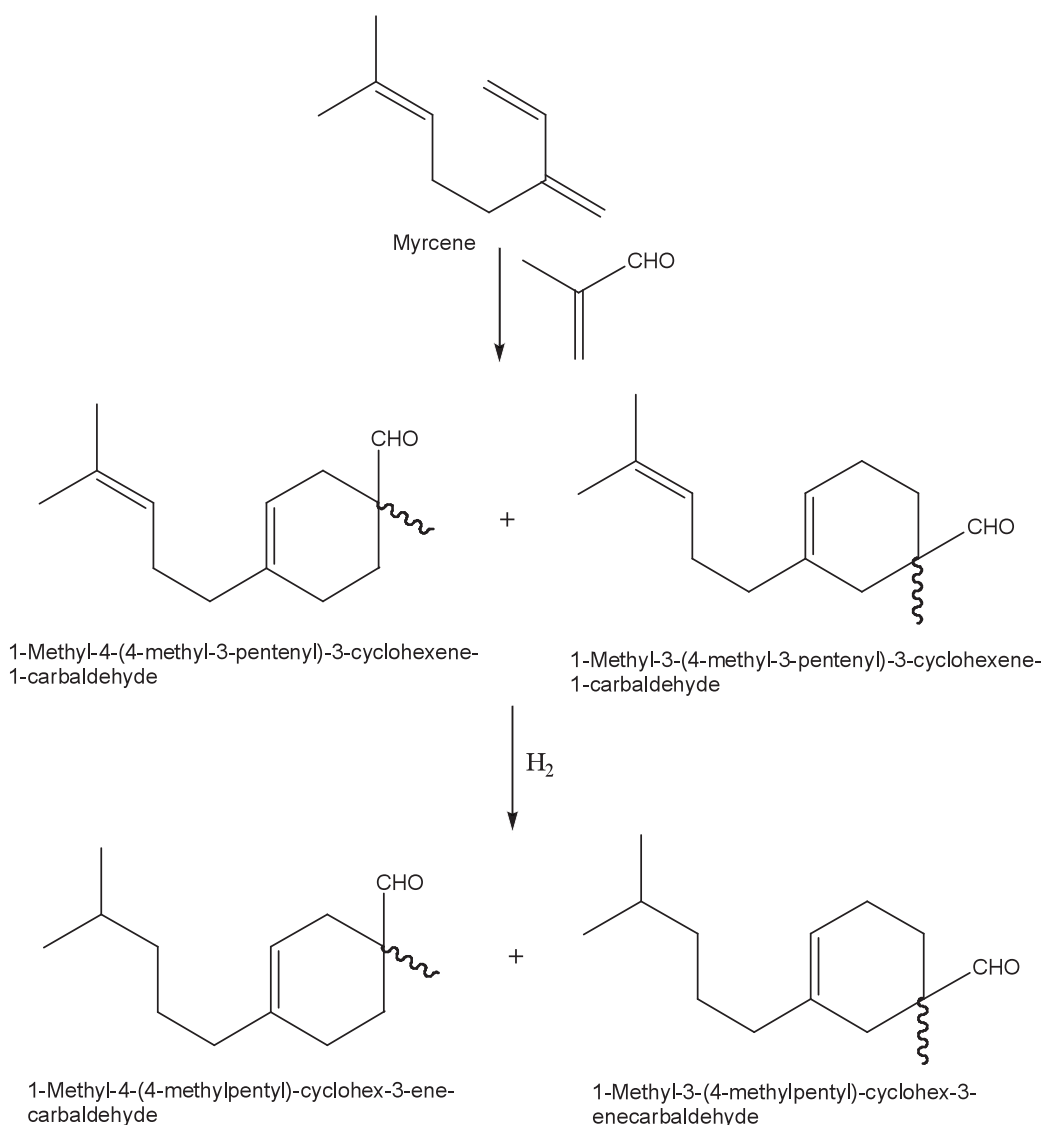
1-Methyl-4-(4-methylpentyl)cyclohex-3-ene-1-carbaldehyde

F-4



Physical data for 1-methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde

CAS#	52475-86-2
Synonym	<i>Precyclemone B</i>
Appearance	Colorless to pale yellow liquid
Molecular weight	206.3
Molecular formula	C ₁₄ H ₂₂ O
Refractive index n _D ²⁰	1.483–1.488
Specific gravity D ₂₅ ²⁵	0.914–0.922
Solubility in alcohol (80 vol. %)	1:4 to 1:10 v/v
Log Po/w	5.19



Physical data for 1-methyl-4-(4-methylpentyl)cyclohex-3-ene-1-carbaldehyde

CAS#	66327-54-6
Synonym	<i>Vernaldehyde</i>
Appearance	Colorless to pale yellow liquid
Molecular weight	208.3
Molecular formula	$C_{14}H_{24}O$
Refractive index n_{20}^D	1.463–1.467
Specific gravity D_{25}^{25}	0.887–0.892
Log Po/w	5.20
Vapor pressure	0.0107 hPa

1-Methyl-4-(4-methyl-3-pentenyl)cyclohex-3-ene-1-carbaldehyde can be synthesized by Mannich reaction of myrcene and 2-methylpropenal, which is produced in situ from formaldehyde, diethylamine and propanal. Selective hydrogenation of the non-cyclic double bond gives 1-methyl-4-(4-methylpentyl)cyclohex-3-ene-1-carbaldehyde, as shown in **F-5**.

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