

Ethyl Dehydrocyclogeranate

Use in fabric, home and personal care, and in fine fragrances

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Ethyl dehydrocyclogeranate (**F-1**), commonly known as ethyl safranate, is a colorless to pale-yellow liquid. It is a mixture of three isomers—2,6,6-trimethylcyclohexa-2,4-diene carboxylic acid ethyl ester (α -isomer), 2,6,6-trimethylcyclohexa-1,3-diene carboxylic acid ethyl ester (β -isomer) and 6,6-dimethyl-2-methylenecyclohexa-3-ene carboxylic acid ethyl ester (γ -isomer) (see **F-2**).

The odor of ethyl dehydrocyclogeranate is described as intense and diffusive, with natural, fresh, damascone, rose and apple notes, woody aspects and longlastingness.^b Ethyl dehydrocyclogeranate is a multifaceted diffusive spicy rose with apple cider and other spicy aspects. This rich ingredient is used in a wide range of fragrance types, from floral to fruity, particularly apple. Ethyl dehydrocyclogeranate gives body and radiance in fine fragrance and toiletries, but is also unexpectedly stable in detergents, thus broadening the possibilities for use in fabric, home and personal care, and in fine fragrances.

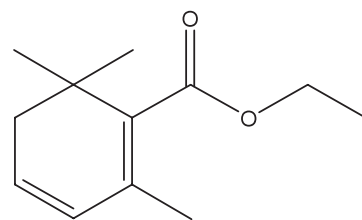
Ethyl 2,6,6-trimethyl cyclohexa-1,3-ene-1-carboxylate;^a ethyl safranate^a;
CAS# 35044-57-6.

^aEthyl safranate is the name used by Givaudan.

^bSome of the information on organoleptic properties and uses are taken from: PMP 96, *Database of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, Netherlands. A few are cited from suppliers' specification sheets, i.e. Givaudan.

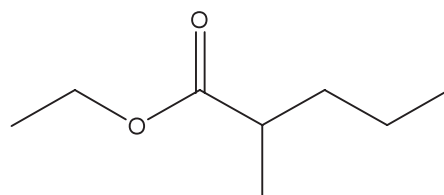
Ethyl dehydrocyclogeranate

F-1



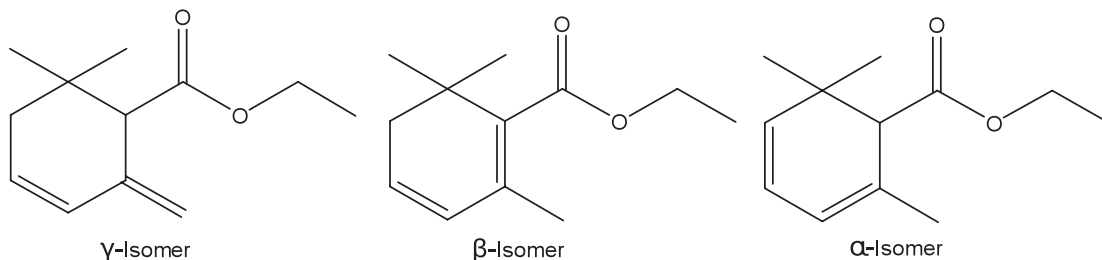
Ethyl 2-methylpentanoate; Manzanate

F-3



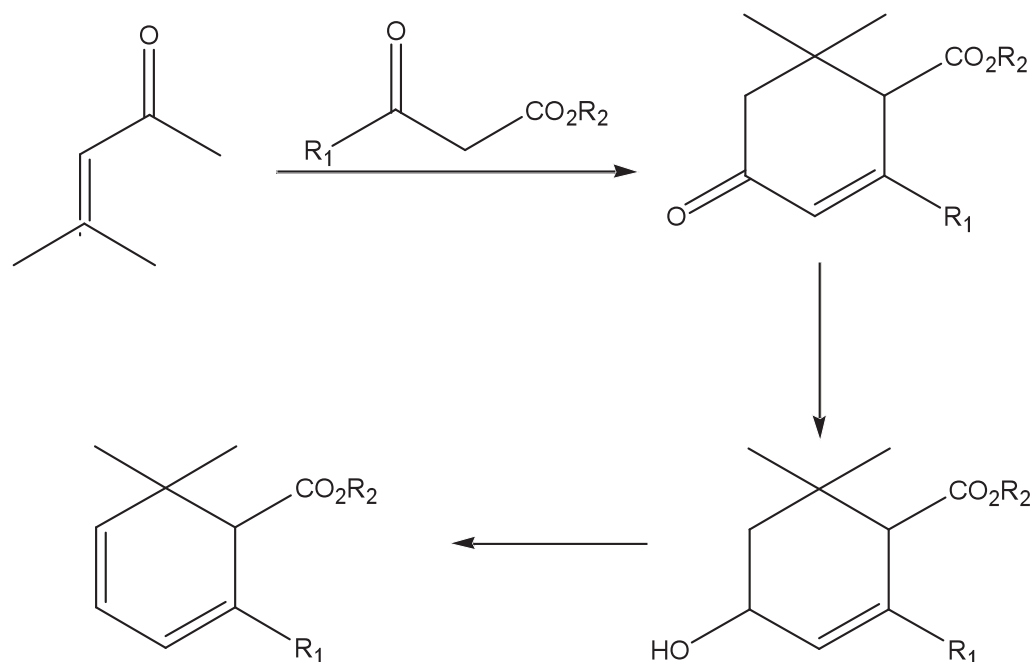
The isomers comprising the mixture ethyl dehydrocyclogeranate

F-2



Ethyl dehydrocyclogeranate is synthesized* by cyclization of mesityl oxide and ethyl acetoacetate, followed by reduction of the carbonyl and elimination of water

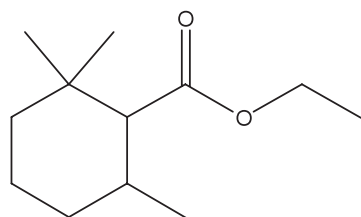
F-4



* GB Pat. 1456162, 1974, and US Pat. 4144199, 1979, and patents cited therein, both assigned to Naarden International BV.

2,2,6-Trimethyl cyclohexane carboxylic acid ethyl ester; Thesaron

F-5



Physical Data for Ethyl Dehydrocyclogeranate

Appearance: colorless to pale yellow liquid

Molecular weight: 194.3

Molecular formula: $C_{13}H_{18}O_2$

Refractive index (20°C): 1.474–1.480

Relative density (D₂₀/4): 0.962–0.972

Flash point: 85°C (closed cup)

Log P: 4.2

The material shows good tenacity, reasonable alkali stability, but performs less well in liquid bleach and acidic cleaner liquid. The best pH ranges to use are 3–10. The material's substantivity lasts several days, and the recommended use level is ca. 2%.

Due to its strongly herbal-fruity, slightly floral, and boiled apple note, ethyl dehydrocyclogeranate may be applied in aromatic, fruity-herbal formulations, e.g. apple-sauce. However, the material has not yet been reported as being found in nature, though it probably exists in saffron. The ingredient does not have a FEMA number and thus is not commonly used in flavors.

During "Fragrance: Scents of Direction" at the British Society of Perfumers' 2006 Symposium, ethyl safranate was presented as a spicy rose with apple cider. This material has been used with *Rosa damascena* oil and is said to give body and diffusivity in fine fragrance—even though it is not typically used in this area—and is a strong performer in technical perfumery. The material has a slight herbal note, but the supplier insists this should not deter people from using it. It is said to combine well with ethyl 2-methylpentanoate (F-3; Manzanate) to lift performance, and has performed very well in a consumer survey.^c It is particularly popular in Japan, where it is used in a number of products at high levels.

^cManzanate is a trade name of Givaudan.

Ethyl dehydrocyclogeranate is synthesized by cyclization of mesityl oxide and ethyl acetoacetate, followed by reduction of the carbonyl and elimination of water (**F-4**).^d

An interesting derivative of ethyl dehydrocyclogeranate is Thesaron (2,2,6-trimethyl cyclohexane carboxylic acid ethyl ester; **F-5**).^e

Thesaron has the fruity-rosy note of a very expensive class of molecules called rose ketones.

According to perfumer and author Arcadi Boix Camps, ethyl safranate is a beautiful ingredient, but unstable compared with Thesaron, which is stable even in bleach.¹

^dGB Pat. 1456162, 1974, and US Pat. 4144199, 1979, both assigned to Naarden International BV.

^eThesaron is a trade name of Takasago.

References

1. A Boix Camps, *Fragrance Creation: Gardenia in Perfumery*. *Perfumer Flavorist*. **33**, 28–33 (2008).

Errata

A typo in **F-3**, appearing on **Page 23** of the October 2010 issue, misidentifies the structure as 2,5-dimethyl-5-heptanal; the material in fact is 2,6-dimethyl-5-heptanal. We regret the error.

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