

# Pear Ester: Ethyl (E,Z)-2,4-decadienoate

Chemistry and application in fragrance and flavor

Michael Zviely, CIC; mzviely@cathay-israel-chemistry.com

**E**thyl (E,Z)-2,4-decadienoate (FEMA# 3148, CAS# 3025-30-7), or pear ester (**F-1**), is a colorless liquid with a highly intense green odor, which occurs naturally in apple, Bartlett pear, Concord grape, beer, pear brandy and quince. It has a green, fruity, apple odor, with tropical nuances and a juicy, ripe pear, sweet, very fruity flavor. The ester's uses in flavors include fruity red, fruity yellow, fruity tropical and other fruity applications. In fragrances, its uses encompass fruity compounds for alcoholic and cosmetic perfumes.

Ethyl (E,Z)-2,4-decadienoate is prepared from *cis*-1-heptenyl bromide, which is converted to 1-heptenyl lithium cuprate complex with lithium and copper iodide.<sup>1</sup> Further reaction of the lithium cuprate complex with ethyl propiolate yields a mixture of isomeric esters (**F-2**). The product is not pure and contains min. 92% of the 2E,4Z-isomer (**F-3**).

Ethyl (E,Z)-2,4-decadienoate is also prepared by enzymatic esterification of other (2E,4Z)-deca-2,4-dienoate esters with lipase obtained from *Candida antarctica* in the presence of ethanol.<sup>2</sup>

Ethyl (E,Z)-2,4-decadienoate is also used in blackcurrant odorants, which are powerful materials. For example, a blackcurrant note joins the pear-musk theme in *Courreges 2020* (Andre Coureges, 1997). In this perfume, the pear note is mainly a consequence of about 5% of ethyl (2E,4E)-deca-2,4-dienoate. Pear ester is another version of the simple ester hexyl acetate (FEMA# 2565, CAS# 142-92-7) (**F-4**), having a sweet, fruity, estery odor similar to pear.

Hexyl acetate was first introduced to the market in personal hygiene products such as L'Oreal's *Elsève Alpha Joboba*, a shampoo introduced in 1995.<sup>3</sup> In *Tempore*



*Donna* (Laura Biagiotti, 1999), hexyl acetate was used in a pear-chocolate accord that was blended with vanilla.<sup>4</sup>

The pear odors have become increasingly fashionable in odorants within the last decade, and they continue to grow in popularity. Pear nuances have recently become trendy in feminine perfumes, playing sensually with musky notes, and the popularity of these odorants spawned a search for other novel pear-scented compounds.

Anapear<sup>a</sup>, or octa-4,7-dienoic acid methyl ester (CAS# 189440-77-5), was discovered by Roman Kaiser of Givaudan and is prepared by the Johnson ortho-ester variant of the Claisen rearrangement (**F-5**). It is used, for example, in *Emporio Armani Elle* (G. Armani, 1998).

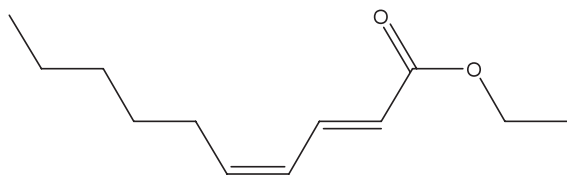
Another fine pear odorant is Pearlate<sup>b</sup>, or 3(Z)-octenyl propionate (FEMA# 4189, CAS# 94134-03-9) (**F-6**). It has a unique soft musk with a pear-apple character drying down to the pulpiness of honeydew melon with cantaloupe and artichoke undertones. It is used for a sweet prickly pear note in floral accords and exotic fragrances and as a good addition to pear flavors to distinguish them

<sup>a</sup> Anapear is a registered trade name of Givaudan.

<sup>b</sup> Pearlate is a registered trade name of Bedoukin Research.

Ethyl (E,Z)-2,4-decadienoate

**F-1**



## Physical Data Ethyl (E,Z)-2,4-decadienoate

Appearance: colorless liquid

Molecular weight: 196.3

Molecular formula: C<sub>12</sub>H<sub>20</sub>O<sub>2</sub>

Refractive index n<sup>20</sup>/D: 1.480–1.486

Specific gravity D<sup>20</sup>: 0.917–0.920

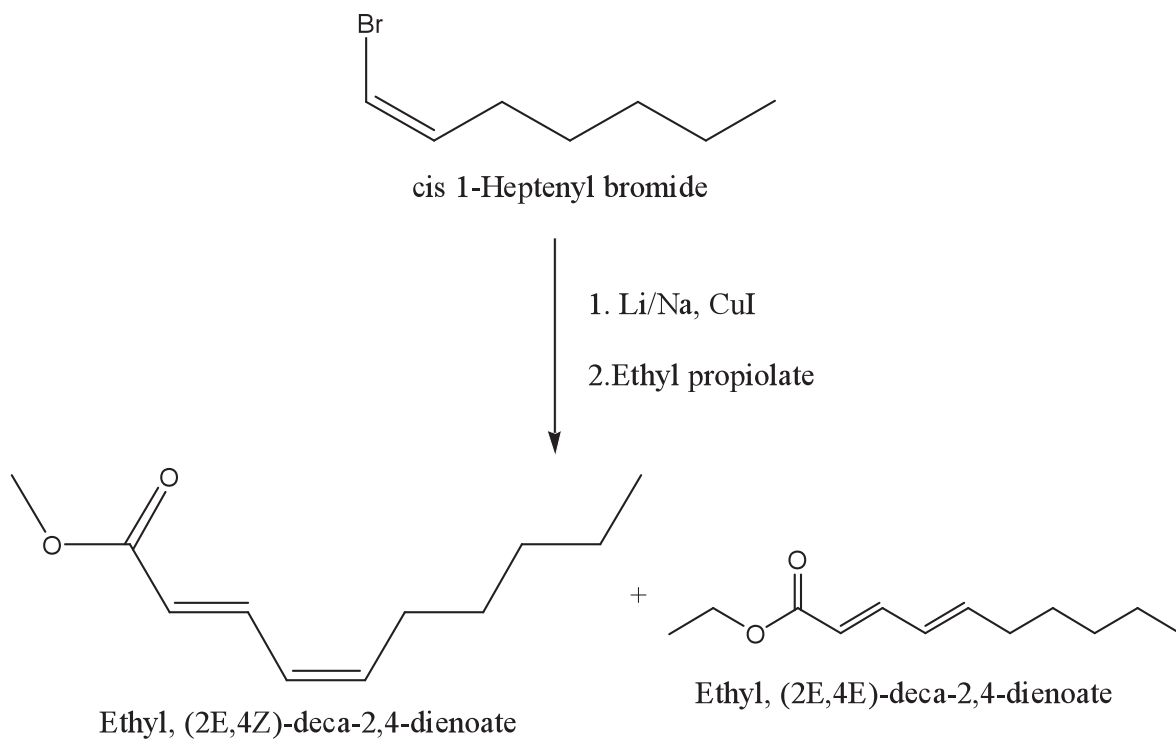
Boiling point: 70–72°C (0.05 mmHg)

Flashpoint: <110°C

LogP: 4.52 (estd.)

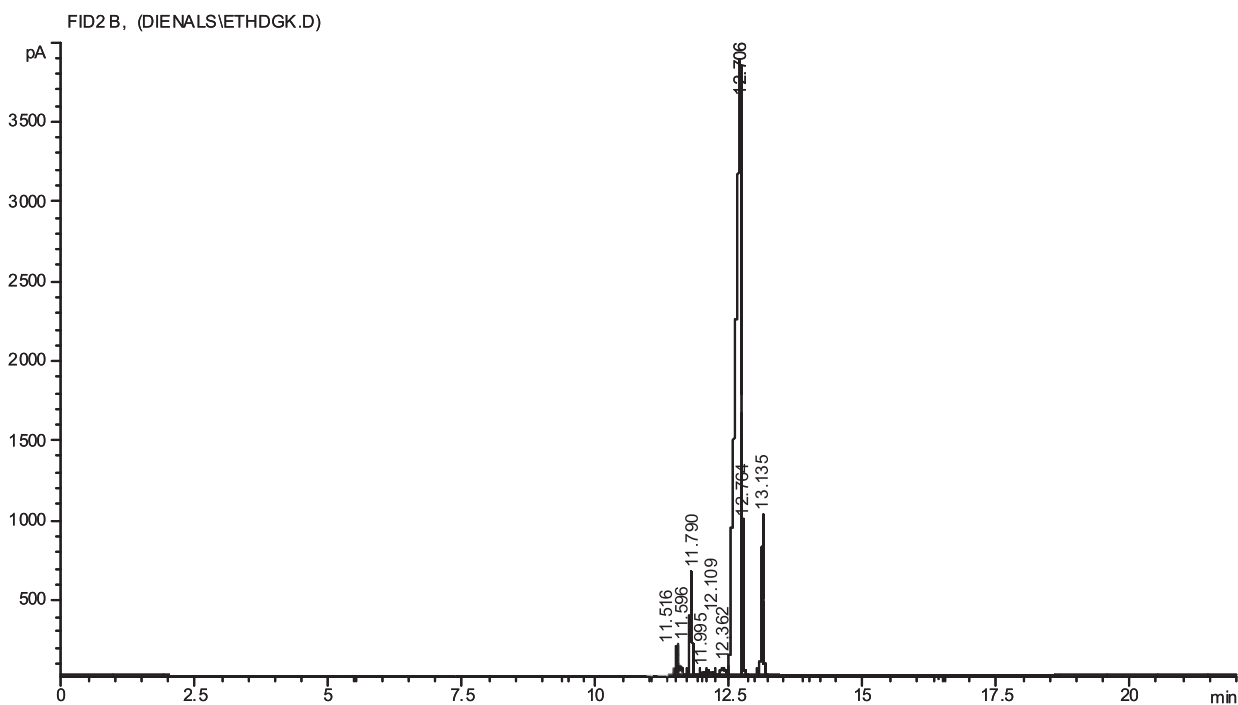
*cis* 1-Heptenyl bromide converted to 1-heptenyl lithium cuprate complex with lithium and copper iodide; further reaction of lithium cuprate complex with ethyl propiolate for a mixture of isomeric esters

F-2



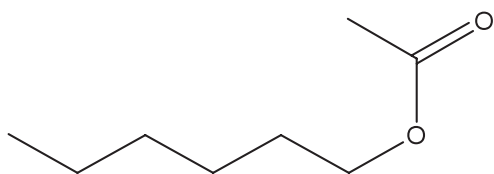
Typical GC of ethyl (E,Z)-2,4-decadienoate

F-3



Hexyl acetate

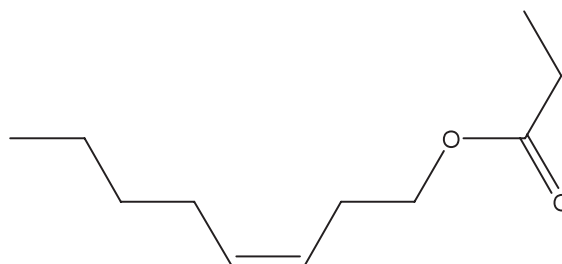
F-4



Hexyl acetate

(Z)-3-Octenyl propionate

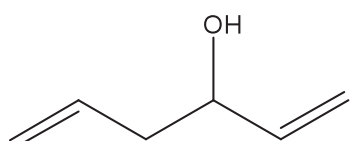
F-6



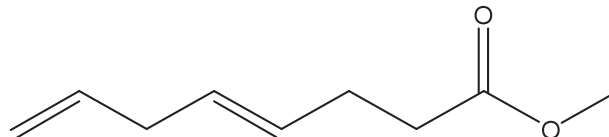
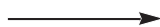
(Z)-3-octenyl propionate

Johnson ortho-ester variant of the Claisen rearrangement preparation of octa-4,7-dienoic acid methyl ester

F-5



Hexa-1,5-dien-3-ol



Octa-4,7-dienoic acid methyl ester

from apple or banana. It is also suitable for melon and grape flavors.<sup>c</sup>

Additionally, studies on the impact of ethyl (E,Z)-2,4-decadienoate on the behavior of newly hatched codling moth *Cydia pomonella* (L.) larvae were also conducted. In general, on apple and pear fruits treated with pear ester, the number of *C. pomonella* larvae that entered the fruit was lower than on untreated fruits, and so was the damage caused by the larvae. These effects are of potential importance for direct applications of pear ester in *C. pomonella* control strategies, especially for improving the efficacy of larvicidal insecticides.<sup>5</sup>

<sup>c</sup> Bedoukian Research Institute specification sheet.

#### References

1. N Ferdinand, *Utilisation de Composés Carbonylés Insaturés Comme Agents Parfumants*, CH 544803, assigned to Firmenich (1973).
2. I Gatfield and G Kindel, *Process for the Preparation of trans-2, cis-4-Decadienic acid ethylester*. EP 0770685, assigned to Haarman & Reimer (1997).
3. N Shah, *Fragrance Chemistry Seminar*, University of Wisconsin, Madison (2001).
4. P Kraft, JA Bajgrowicz, C Denis and G Frater, *Angew Chem Int Ed*, **39**, 2980–3010 (2000).
5. E Pasqualini, M Villa, S Civolani, I Espinha, C Ioriatti, S Schmidt, F Molinari, A De Cristofaro, B Sauphanor and E Ladurner, *Bull Insect*, **58**(1), 65–69 (2005).