

The Passion Fruit Core: 2-Methyl-4-propyl-1,3-oxathiane

Chemistry and application in fragrance and flavor

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2-Methyl-4-propyl-1,3-oxathiane (FEMA# 3578, CAS# 59323-76-1, CAS# 67715-80-4) (**F-1**) is a colorless to pale yellow liquid with an extremely powerful olfactory impact, a tropical green passion fruit note and a grapefruitlike tartness.

2-Methyl-4-propyl-1,3-oxathiane occurs naturally in yellow passion fruit juice. Its uses in flavors are mostly in exotic fruit formulations such as citrus fruits, passion fruit and tropical fruits. In fragrances, it is good in citrus and exotic fruity notes and brilliant in jasmine and rose and muguet florals, as well as in green aldehydic perfumes. Traces of 2-methyl-4-propyl-1,3-oxathiane will add unique effects to any fragrance creation.^a

2-Methyl-4-propyl-1,3-oxathiane has four isomers, of which two occur in nature (**F-2**), and it is prepared from leaf aldehyde (*trans*-2-hexenal) in a three-stage process¹ (**F-3**). The material can be applied to fine fragrances, shower gels, shampoos, detergents, soaps, candles and softeners in traces up to 0.1%.

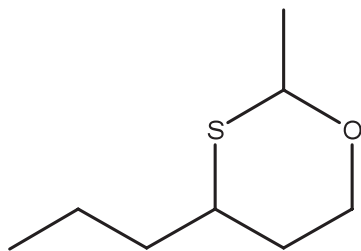
2-Methyl-4-propyl-1,3-oxathiane also is used in black-currant odorants, which are powerful materials, and for this reason are used in the form of perfumery base; for example, it is in the green, fruity, floral, fresh base of

^a Information taken from Firmenich, Givaudan, Frutarom and Symrise specification sheets, and FRM 2001 *Database of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, The Netherlands.



2-Methyl-4-propyl-1,3-oxathiane (galbanum oxathiane, Oxane^b, Trophathiane^c, Oxanthia^d)

F-1



^b Oxane is a trade name used by Firmenich.

^c Trophathiane is a trade name used by Frutarom.

^d Oxanthia is a trade name used by Symrise.

Physical Data for 2-Methyl-4-propyl-1,3-oxathiane

Appearance: Colorless to pale yellow liquid

Molecular weight: 160.3

Molecular formula: C₈H₁₆OS

Refractive index (n_D²⁰): 1.475–1.485

Specific gravity (D₂₀²⁰): 0.971–0.981

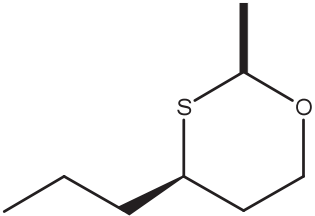
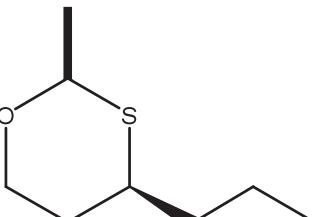
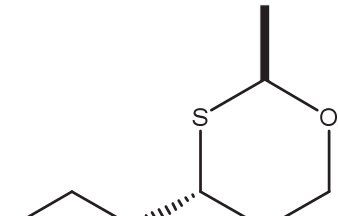
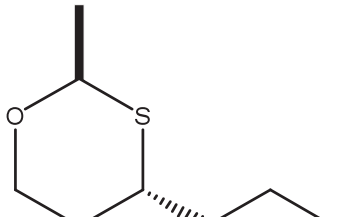
Boiling point: 218–220°C

Flash point: 50°C

LogP: 2.31 (estd.)

Isomers of 2-methyl-4-propyl-1,3-oxathiane

F-2

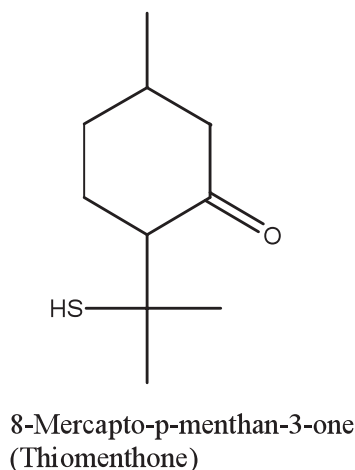
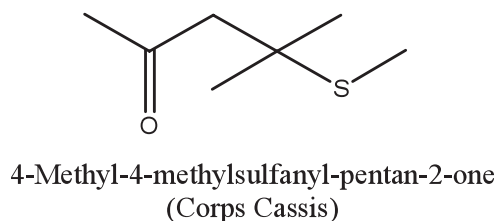
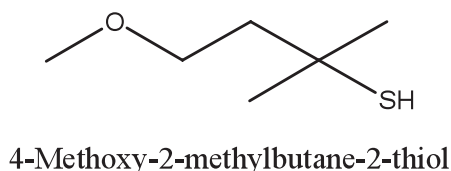
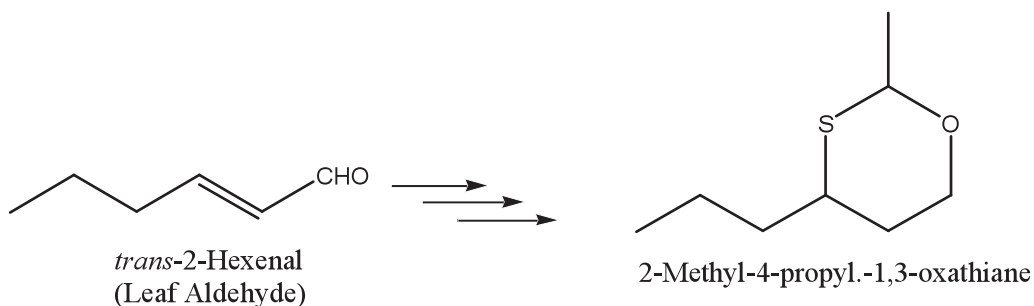
 <p>(2S,4R)-(+)-cis-</p>	<p>Sulfurous, fatty, fruity-green, tropical fruits, grapefruit</p> <p>ϕ value[°] = 8.01E+07</p>
 <p>(2R,4S)-(-)-cis-</p>	<p>Sulfurous, herbaceous-green, fresh, floral, roasty, linseed oil-like, onion; less sulfury than the 2S,4R-isomer</p> <p>ϕ value = 4.01E+07</p>
 <p>(2S,4S)-(+)-trans-</p>	<p>Sulfurous, slight bloomy-sweet</p>
 <p>(2R,4R)-(-)-trans-</p>	<p>Green grass, root, earthy, red radish note</p>

[°] ϕ value = (Odor Threshold X 1000)/MW

Vert de Cassis Givco 180,[°] which features notes of crushed blackcurrant leaves. These bases are easy to work with when they are in even higher concentration. For instance, about 18% of cassis bases were employed in the floral-fruity feminine fragrance *Le Monde est Beau* from Kenzo, described by the company as the fragrance of happiness and joy of living, an echo of nature and a source of life.²

[°] Vert de Cassis Givco 180 is a trade name of Givaudan.

Other blackcurrant ingredients include 2-methoxy-2-methylbutane-2-thiol (FEMA# 3785, CAS# 94087-83-9), 4-methyl-4-methylsulfonyl-pentan-2-one (FEMA# 3376, CAS# 23550-40-5) and thiomenthone (FEMA# 3177, CAS# 38462-22-5) (**F-4**). 2-Methoxy-2-methylbutane-2-thiol has a characteristic sulfur note of blackcurrant with an extremely high ϕ value of 2.98E+15. This material is responsible for the catty, fruity sensory properties and sulfurous note found in blackcurrant buds. Traditionally,




buchu oil and thiomenthone have been used to achieve this type of note in the formulation of blackcurrant flavors. It is also used in other fruit flavors, such as tropical fruit and peach.^f

4-Methyl-4-methylsulfonyl-pentan-2-one odor is sulfurous, with horseradish, fried garlic, green, fruity and blackcurrant notes at high dilution. In flavors, it is used in bakery and soft confection at 2 ppm and in frozen dairy, meat products, desserts and beverages at 1 ppm.

Thiomenthone odor is blackcurrant, buchu, herbaceous and minty. Its usage in flavors is in alcoholic beverages, apricot, blackcurrant, herbal flavors, mango, pineapple, and soft and tropical fruits.

References

1. W Pickenhagen and H Bronner-Schindler, *Helv Chim Acta*, **87**, 947–952 (1984); A Mosandl and G Heusinger, *Liebigs Ann Chem*, 1185–1191 (1985); G Singer, G Heusinger, O Frohlich, P Schreier and A Mosandl, *J Agric Food Chem*, **34**(6), 1029–1033 (1986); G Ohloff, *Scent & Fragrances*, 43, Springer-Verlag (1994); MH Boelens, H Boelens and L J van Gemert, *Perfumer & Flavorist*, **18**(6), 1–15, (1993); JC Leffingwell, *Chirality & Odour Perception*, www.leffingwell.com/chirality/chirality.htm.
2. P Kraft, JA Bajgrowicz, C Denis and G Frater, *Angew Chem Int Ed*, **39**, 2980–3010 (2000).

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^f Information taken from Treatt.