Allyl Fragrance and Flavor Ingredients—From Floral-Rosy to Green Onion

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The family of chemicals containing allyl groups is important both to the human sense of smell and taste, and to the fragrance and flavor business community at large. Regardless of whether the resulting compound is aliphatic or aromatic, alicyclic or containing heteroatoms, this short (three-atom) carbon chain seems to contribute a structural olfactophore. The organoleptic span of allyl-containing ingredients covers the range between green and galbanum fruity notes, from floral-rosy to herbal to spicy to pungent, garlicky and green onionlike with meaty nuances.

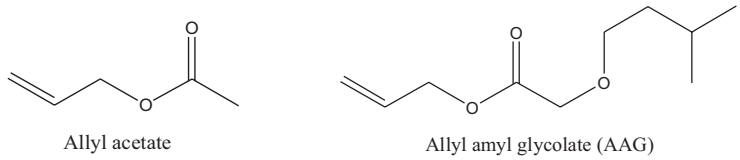
First in this category are the simple aliphatic esters, such as allyl acetate (CAS #591-87-7), which have a diffusive, pungent, gassy odor that is fruity on dilution, and allyl amyl glycolate (**F-1**; AAG; CAS #67634-00-8), a strongly fruity material with a green, herbal odor, galbanum connotations, and apple and pineapple notes[a].

The allyl group can also be connected to an alicyclic ester, as in the case of allyl cyclohexane acetate (CAS #4728-82-9), which results in a sweet, ripe, pineapple-like odor with a green waxy nuance. Allyl cyclohexane propionate (CAS #2705-87-5), a fruity, pineapple, waxy odor with green sweet apple nuances, is another example in this series (**F-2**).

Aromatic allyl esters can be represented by two artificial ingredients: allyl cinnamate (CAS #1866-31-5), which has balsamic and peach notes, and allyl anthranilate (CAS #7493-63-2) which has a sweet aromatic, somewhat citrusy, tangerinelike odor (**F-3**).

If a cyclohexane ring is connected to the allyl group via an ester-ether bridge, the result is a molecule like allyl cyclohexyl glycolate (**F-4**; also called allyl cyclohexyl

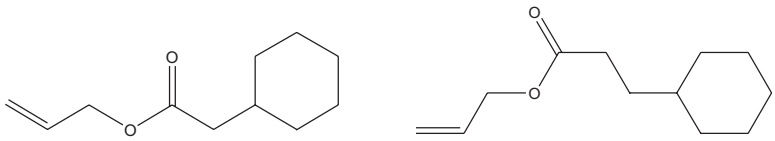
Allyl acetate and allyl amyl glycolate **F-1**



Allyl acetate

Allyl amyl glycolate (AAG)

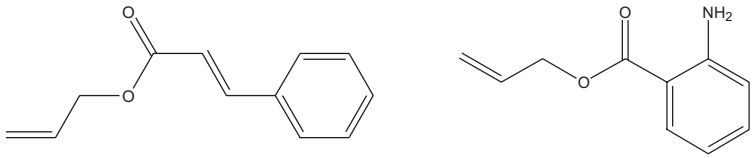
Allyl cyclohexane acetate and allyl cyclohexane propionate **F-2**



Allyl cyclohexane acetate

Allyl cyclohexane propionate

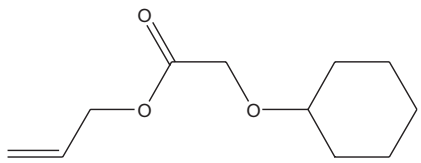
Allyl cinnamate and allyl anthranilate **F-3**



Allyl cinnamate

Allyl anthranilate

Allyl cyclohexyl glycolate (allyl cyclohexyl oxyacetate) **F-4**

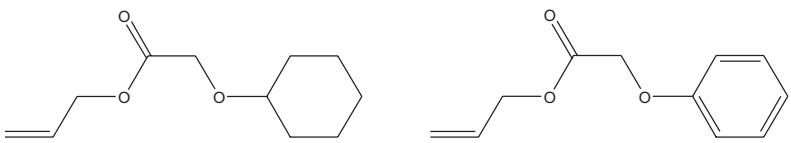


C11H18O3 CAS# 68901-15-5

Sold as: Cyclogalbanate, Cyclogalbaniff (IFF trade name), galbador CG

[a] Most of the information on organoleptic properties and uses is taken from *e.g.* FRM 2001 and PMP 96 *Databases of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, The Netherlands.

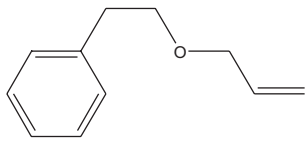
Allyl cyclohexyl oxyacetate and allyl pheonxyacetate **F-5**



Allyl cyclohexyloxy acetate

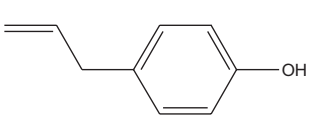
Allyl phenoxy acetate

Allyl phenylethyl ether **F-6**

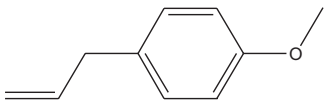


Allyl phenylethyl ether

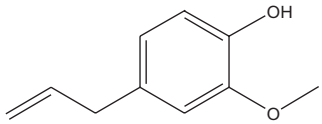
4-Allylphenol, 4-allylmethoxybenzene and 2-methoxy-4-allylphenol **F-7**



4-Allylphenol



4-Allylmethoxybenzene



2-Methoxy-4-allylphenol

oxyacetate; CAS #68901-15-5), a bright galbanum, pineapple-scented material with green, leafy, watery, metallic, berry[b] and cool dry-spicy nuances[c].

The aromatic companion molecule to allyl cyclohexyl glycolate is allyl phenoxyacetate (CAS #7493-74-5), an artificial aroma with a sweet, pineapple, honey odor (**F-5**).

Allyl alcohol can be directly connected by an ether function, as in the case of allyl phenylethyl ether (CAS #14289-65-7), a fresh, sweet, aromatic, floral ingredient suggestive of rose and chamomile (**F-6**).

[b] IFF spec. sheet
[c] Symrise data sheet

Physical Data for Allyl cyclohexyl glycolate

Appearance:	Colorless to pale yellow liquid
M.W.:	198.26
Specific Gravity:	1.0120 to 1.0200 25°C
Refractive Index:	1.4600 to 1.4640 20°C
Flash Point:	>100°C TCC (>212°F)
logP (o/w):	2.96 (estd.)

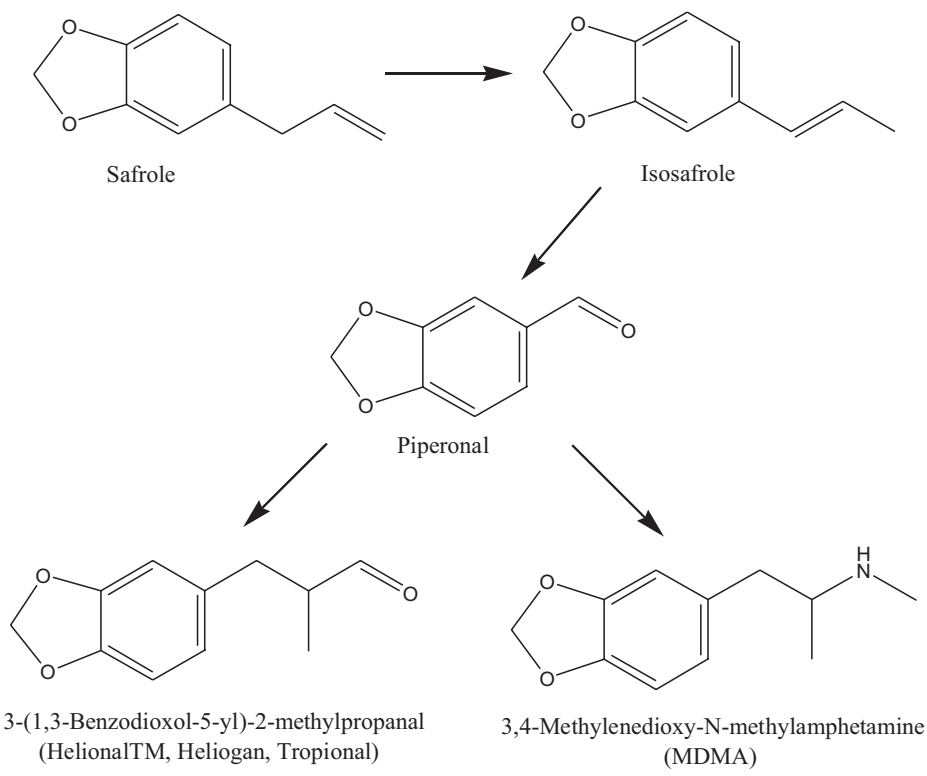
The allyl group can also "hang off" a larger molecule. For example, it can be directly connected to a benzene ring by a carbon-carbon bond, which results in 4-allylphenol (chavicol; CAS #501-92-8), an aromatic spicy, somewhat medicinal phenolic compound; 4-allyl methoxybenzene (estragole; CAS #140-67-0), a sweet, spicy chemical with a scent characteristic of sweet basil and licorice; or 2-methoxy-4-allylphenol (eugenol; CAS #97-53-0), a molecule with a warm, spicy, clovelike odor (**F-7**).

Sassafras oil (*Sassafras albidum*) is the source of another allyl-containing molecule (and MDMA component), safrole (CAS #94-59-7), which is an important starting material for 3-(1,3-benzodioxol-5-yl)-2-methylpropanal (known as helional, heliolan and Tropional [Vigon trade name]); CAS #1205-17-0).[1] Safrole can be isomerized into isosafrole (CAS #120-58-1) and then further oxidized to give piperonal (heliotropine; CAS #120-57-0). Piperonal can also can be used to form the psychoactive drug 3,4-methylenedioxy-N-methylamphetamine (MDMA; CAS #42542-10-9)[d], a regulated compound (**F-8**).

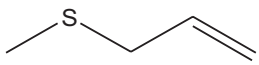
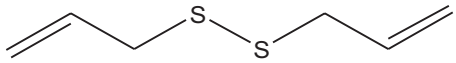
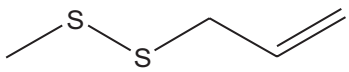
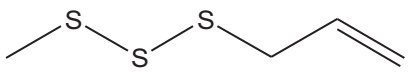
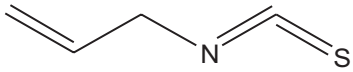
Sulfur derivatives are a completely different group of allyl-containing ingredients, several examples of which are shown in **F-9**.

[d] MDMA is legally controlled in most of the world under the UN Convention on Psychotropic Substances and other international agreements, although exceptions exist for research. In general, the unlicensed use, sale or manufacture of MDMA is a criminal offense.

Safrole can be used to produce both 3-(1,3-benzodioxol-5-yl)-2-methylpropanal and the psychoactive drug 3,4-methylenedioxy-N-methylamphetamine, or MDMA, a regulated compound **F-8**

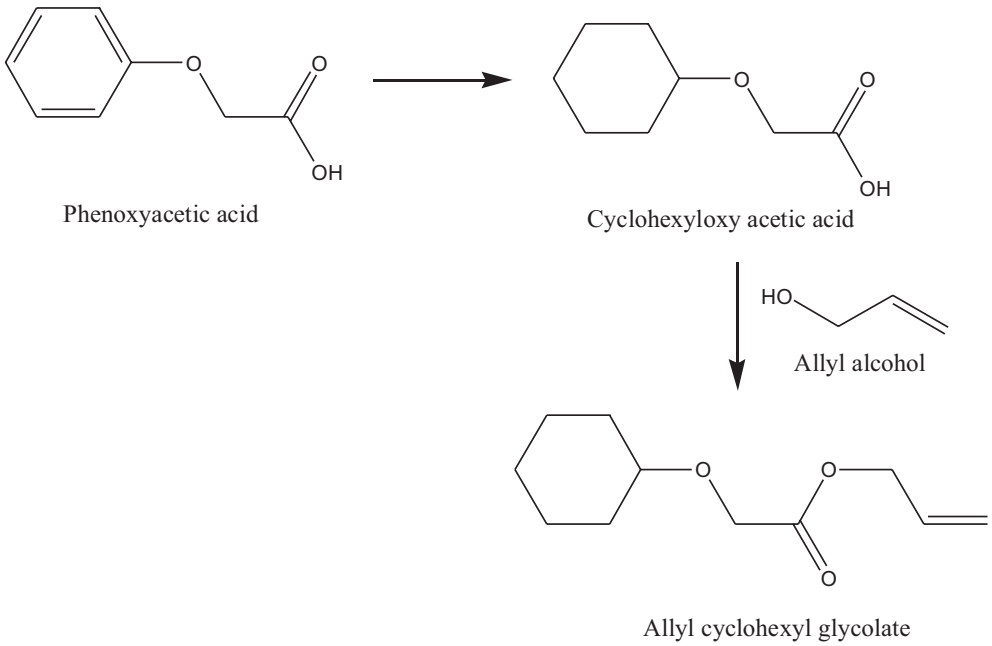


Several examples of sulfur derivatives **F-9**

MATERIAL CAS No.	STUCTURE	ORGANOLEPTIC CHARACTERISTICS
Allyl methyl sulfide[2] (CAS #10152-76-8)		Sulfuraceous, allium
Allyl disulfide (CAS #2179-57-9)		Pungent, alliumlike, garlic; green onionlike with meaty nuances
Allyl methyl disulfide (CAS #2179-58-0)		Pungent, alliciaceous; clear note of garlic on dilution
Allyl methyl trisulfide (CAS #34135-85-8)		Strong, alliumlike; note of garlic and leek
Allyl isothiocyanate[3] (CAS #57-06-7)		Pungent, sharp, characteristic mustardlike; vegetable note on dilution

Synthesis of allyl cyclohexyl glycolate

F-10



To synthesize the title compound, phenoxyacetic acid is hydrogenated to cyclohexyloxy acetic acid, then further reacted with allyl alcohol to obtain allyl cyclohexyl glycolate (**F-10**). This compound can be used in fine fragrance formulations. It is a principle component of *Eau de Magnolia* by Arcadi Boix Camps, in which it is combined with floral ingredients such as ethyl linalool, Floralozone (IFF trade name), Bourgeonal (original Quest trade name) and Lilial (Givaudan trade name).[4] Glen Brechbill has formulated a rose compound, called *Rosa Gallica Pontiana*, with allyl cyclohexyl glycolate, by adding geraniol, linalool and isojasmone.[5]

References

1. M Zviely, The Phenylpropanals—Floral Aromatic Aldehydes, *Perfum Flavor*, 37, 52 (2012)
2. DJ Rowe, Aroma Chemicals for Savory Flavors, *Perfum Flavor*, 23, 9 (1998)
3. M Zviely, The Universal Hotness—Part I, *Perfum Flavor*, 36, 66 (2011)
4. A Boix-Camps, *Perfum Flavor*, 32, 46, 2007
5. GO Brechbill, *Arranging Fine Perfumes Compositions—The Rose*, 257, Fragrance Books Inc., New Jersey (2011)