

Molecule of the Month: 5-Isopropyl-2-methylphenol

Organoleptic profile and application areas

Michael Zviely, CIC

5-Isopropyl-2-methylphenol, also known as carvacrol, is one of the three isomers of isopropylmethylphenol. It is a transparent, colorless to pale yellow liquid and the main constituent of origanum oil (see F-1). Carvacrol also occurs in some essential oils of the *Labiata* family such as azov and thyme oils, beer and cranberry.[°] Its odor profile is aromatic, somewhat medicinal, phenolic, spicy, herbal and woody. The other two isomers of isopropyl methylphenol are thymol and *meta*-thymol; all three isomers differ in their organoleptic properties (see F-2).

Carvacrol possesses a penetrating, dry-medicinal (phenolic) and herbaceous odor with a spicy undertone; the lack of sweetness is the differentiating factor between carvacrol and thymol, the former being relatively tarrier. It finds application in aromatic flavorings; spicy and meaty nuances; dill, clove, caraway, smoke and mint notes; oral care products; and tutti frutti. It is used as a flavoring agent in feed, and also possesses antibacterial properties.¹ In addition, carvacrol is used in perfume compositions such as industrial fragrances, certain types of heavy-duty household fragrances and soap perfumes. Despite belonging to the hydroxyl group, this material is powerful and fairly stable in ordinary soaps.

Azov oil is a natural, pale yellow to yellow liquid from the botanical *Origanum syriaca*.^{**} This interesting essential oil contains either up to 80% carvacrol or up to 60% thymol in its various carvacrolic and thymolic types. It possesses a combined organoleptic profile of thyme, marjoram and oregano (see F-3). This essential oil finds application in aromatic flavorings; spicy and meaty nuances; dill, clove, caraway, smoke, mint and cooling notes; oral care products; and tutti frutti. In fragrances, it can be used as a modifier in herbaceous and fougere perfumes, as well as in masculine and spicy notes.^{***}

[°]Most of the information on organoleptic properties and uses is taken from the FRM 2001 and PMP 96 Databases of *Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, Netherlands; and Steffen Arctander's *Perfume and Flavor Chemicals (Aroma Chemicals Vols 1 & 2)* and *Perfume and Flavor Materials of Natural Origin*.

^{**}*Majorana syriaca* L. Feinbrun

^{***} www.perfumerflavorist.com/flavor/rawmaterials/natural/43282897.html



Physical Data

CAS# 499-75-2

FEMA# 2245

CE 2055

Appearance Transparent, colorless to pale yellow liquid

Molecular Weight 150.2

Molecular Formula C₁₀H₁₄O

Refractive Index (20°C) 1.521–1.526

Specific Gravity (25°C) 0.974–0.979

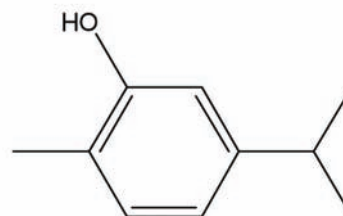
Solubility Soluble in four and more parts of 60% alcohol

Boiling Point 234–236°C

Flash Point (cc) 106°C

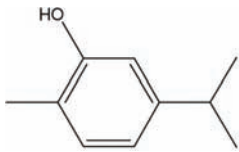
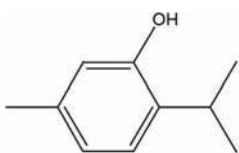
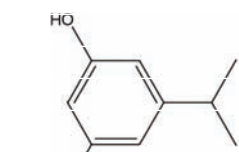
Carvacrol

F-1



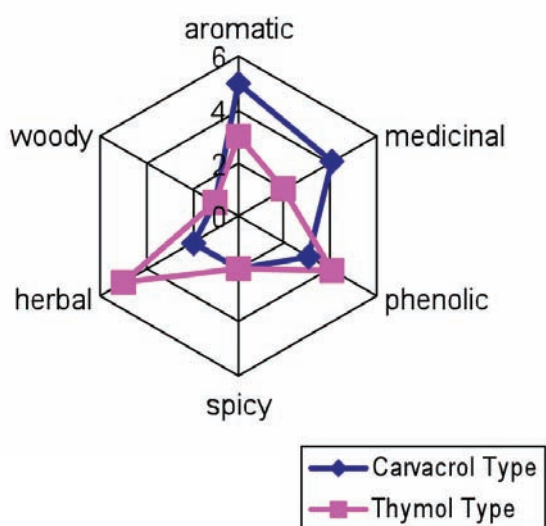
The family of the isopropylmethyl phenols

F-2

Carvacrol		5-Isopropyl-2-methylphenol	Aromatic, somewhat medicinal, phenolic; spicy, herbal, woody
Thymol		2-Isopropyl-5-methylphenol	Spicy, aromatic, characteristic thyme; phenolic, medicinal and woody.
<i>meta</i> -Thymol		3-Isopropyl-5-methylphenol	Weaker, less tarry, more typical phenolic-medicinal.

The organoleptic profile of azov oil types

F-3



Carvacrol can be prepared directly from α -pinene or p-cymene; the standard process, however, uses carvone as starting material (see F-4). Carvacrol can be used as starting material for carvacrol methyl ether (1-methoxy-2-methyl-5-isopropylbenzene), which occurs in many essential oils such as ginger, pepper, thyme, marjoram and savory. It has an aromatic, slightly herbal and somewhat medicinal-phenolic odor profile with a green root connotation. This material is used in spicy and tobacco formulations.

Address correspondence to Michael Zviely, 3, Haim-Hazaz St, Haifa, 34996, Israel; mzviely@cathay-israel-chemistry.com.

References

1. JM Kim, MR Marshall, JA Cornell, JF Preston and CI Wei, Antibacterial activity of carvacrol, citral, and geraniol against *salmonella typhimurium* in culture medium and on fish cubes, *J Food Sci*, 60(6), 1364–1368, 1374 (1995)

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Preparation of carvacrol using carvone as the starting material

F-4

