

# Molecule of the Month: 2,3-Pentanedione

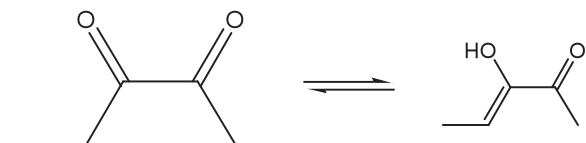
Chemistry and application in butter and dairy, fruit, and roasted flavors

Michael Zviely

2,3-Pentanedione (acetyl propionyl) is a yellow liquid that exists in diketonic form. However, in some GC conditions, 2,3-pentanedione can appear in its enol form, *i.e.* 3-hydroxypent-3-en-2-one, up to a small percentage (see F-1).

## 2,3-Pentanedione in its enol form

F-1



2,3-Pentanedione occurs in butter, bread, milk, yogurt, chicken, meat, cocoa, coffee, potato chips, roasted almonds, pecans, beer, red and white wine, rum and whiskey. The organoleptic profile can be described as creamy, penetrating, cheesy, oily, sweet, buttery, almondlike, brown roasted, and somewhat caramellic, with a fruity nuance.\*

2,3-Pentanedione belongs to the important family of  $\alpha$ -diketones, which includes diacetyl, 2,3-hexanedione (acetylbutyryl), 3,4-hexanedione (dipropionyl), 2,3-heptanedione (acetyl valeryl) and 5-methyl-2,3-hexanedione (acetyl isovaleryl). Acetyl methyl carbinol (acetoin) could be also included in this group of materials.

2,3-Pentanedione is formed in Maillard type reaction by two pathways, one involving glucose carbon atoms (10%) and the other (90%) through the participation of C2'-C3' atoms of l-alanine and a C<sub>3</sub> carbon unit from D-glucose.<sup>1</sup> Natural 2,3-pentanedione is also offered in market (see F-2).

2,3-Pentanedione is applied in dairy, fruity and roasted flavor formulations—including cream, butter, cheese, caramel, butterscotch, berries and rum—and partly as a substitute for diacetyl. It can also be applied in cosmetic compounds for lipstick and other creamy formulations. The material, however, shows poor tenacity, being a rather

small molecule of MW 100, though it is relatively stable in basic conditions. Today, due to the safety issues concerning diacetyl, 2,3-pentanedione is becoming an important ingredient, especially in butter flavors.\*\*

2,3-Pentanedione is prepared by reaction of hydroxyacetone and paraldehyde in the presence of hydrochloric acid, with tetrabutylammonium bromide as catalyst (see F-3).<sup>2</sup> 2,3-Pentanedione is also an important raw material for the preparation of alkyl-substituted pyrazines.

\*\* The US National Institute for Occupational Safety and Health has suggested that diacetyl, when used in artificial butter flavoring (as used in many consumer foods), may be hazardous when heated and inhaled over a long period. This concern is the focus of ongoing litigation in the United States and Europe.

## References

1. VA Yaylayan and A Keyhani, *J Agric Food Chem*, 47 (8), 3280–3284 (1999)
2. US Pat 6720456, S Lambrecht, O Franke and K Zahlmann, Symrise GmbH & Co KG [US] (2004)

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## Physical Data

CAS# 600-14-6

FEMA# 2841

CE 2039

Acetyl propionyl

Appearance: Yellow liquid

Molecular Weight: 100.1

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>

Refractive Index (20°C): 1.402–1.410

Specific Gravity (25°C): 0.952–0.980

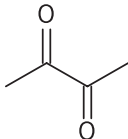
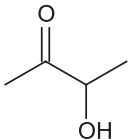
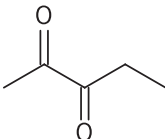
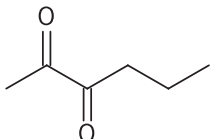
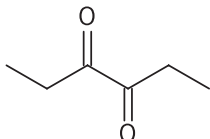
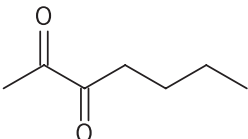
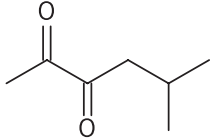
Solubility: Soluble 1 in 3 or more parts of alcohol 50%

Boiling Point: 110–112°C

Flash Point: 18°C (closed cup)

Vapor Pressure (25°C): 3.33KPa

\*Most of the information on organoleptic properties and uses are taken from sources such as FRM 2001 and PMP 96 Databases of Perfumery Materials & Performance, Boelens Aroma Chemicals Information Services, Netherlands.

|                |                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                 |
|----------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 4 Carbon atoms |  <p><b>2,3-Butanedione (diacetyl)</b><br/>Sweet, strongly buttery, creamy, milky</p>                                                                                       |  <p><b>Acetyl methyl carbinol (acetoin)</b><br/>Sweet, buttery, creamy, sour, fatty, vanilla</p>                                                             |
| 5 Carbon atoms |  <p><b>2,3-Pentanedione (acetyl propionyl)</b><br/>Creamy, penetrating, cheese, oily, sweet, buttery, almond, brown roasted, somewhat caramellic, with a fruity nuance</p> |                                                                                                                                                                                                                                                 |
| 6 Carbon atoms |  <p><b>2,3-Hexanedione (acetyl butyryl)</b><br/>Creamy, caramellic, fruity; toasted brown</p>                                                                              |  <p><b>3,4-Hexanedione (dipropionyl)</b><br/>Burnt, caramellic</p>                                                                                           |
| 7 Carbon atoms |  <p><b>2,3-Heptanedione (acetyl valeryl)</b><br/>Buttery, cheesy, oily</p>                                                                                               |  <p><b>5-Methyl-2,3-hexanedione (acetyl isovaleryl)</b><br/>Fresh, fried, roasted and burnt character; slightly fruity; creamy with a pineapple nuance</p> |

