

# Aroma Chemical Profiles

## 3-(4-Ethylphenyl)-2,2-dimethylpropionaldehyde

Michael Zviely

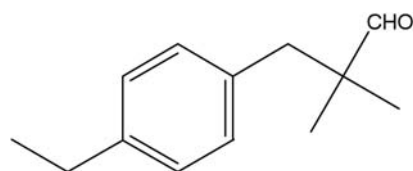


The odor of 3-(4-ethylphenyl)-2,2-dimethylpropionaldehyde is described in part as floral, muguet.

**3**-(4-Ethylphenyl)-2,2-dimethylpropionaldehyde (**F-1**) is a colorless to pale yellow liquid, which exists as the main isomer (60–80%) in the product consisting of an *ortho* isomer (15–35%) and a *meta* isomer (ca. 5%) (**F-2**). It is prepared by condensation of 1-chloromethyl-4-ethylbenzene (tech.) with isobutyraldehyde in the presence of a phase transfer catalyst as shown in **F-3**.<sup>1,2</sup>

The odor of 3-(4-ethylphenyl)-2,2-dimethylpropionaldehyde is described as: floral, muguet, aldehydic, ozonic, powerful, clean, with a fresh air tone reminiscent of ocean breeze.<sup>3</sup> 3-(4-Ethylphenyl)-2,2-dimethylpropionaldehyde (Floralozone, Florazon and Florone) belongs to a family of marine-ozone fragrance ingredients

### 3-(4-Ethylphenyl)-2,2-dimethylpropionaldehyde **F-1**



that includes Precyclemone B, Myrac Aldehyde, Melonal and Helional.<sup>a</sup>

The material shows good tenacity; being a tertiary aldehyde, it is moderately alkali-stable, though not stable at higher temperatures. Its substantivity is greater than two days; the material's recommended use level is ~10%.

### Applications

This aldehyde is applied for a fresh air lift in detergent and cosmetic formulations. Primary recommended uses include alcoholic lotions, antiperspirants, deodorant sticks, fabric softeners, shampoos and soaps. The

<sup>a</sup>Floralozone; Precyclemone B; Myrac Aldehyde; and Helional are trademarks of IFF; Florazon is a trademark of Symrise; Florone is a trademark of O'Laughlin; Melonal is a trademark of Givaudan

### Physical Data

CAS# 67634-15-5

Trade names: Floralozone (IFF), Florazon (Symrise) and Florone (O'Laughlin)

Appearance: Colorless to pale yellow liquid

Molecular weight: 190.3

Molecular formula: C<sub>13</sub>H<sub>18</sub>O

Refractive index (20°C): 1.504–1.510

Relative density (D<sub>20/4</sub>): 0.951–0.959

Flash point: >100°C (closed cup)

Log p: 3.60

ingredient figures prominently in *Vétiver Extraordinaire*, released by Frederic Malle in 2002. The fragrance was created by perfumer Dominique Ropion, according to an official Frederic Malle release, and includes “an overdose” (25%) of vetiver matched to woody notes.

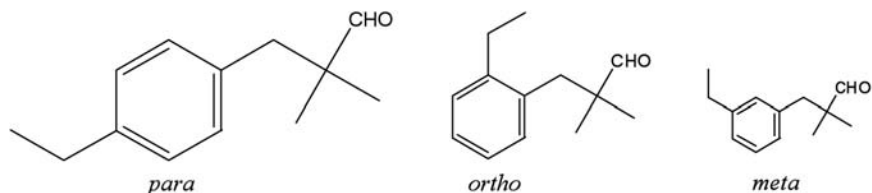
Look for the next installment of *Aroma Chemical Profiles in the July edition of P&F magazine*.

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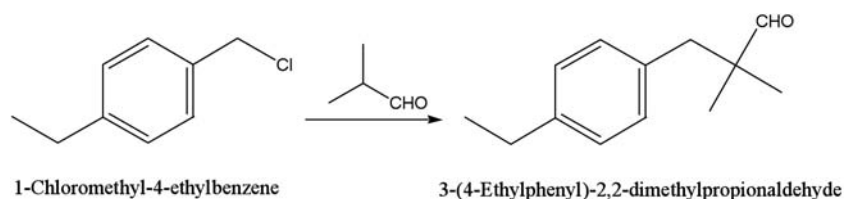
#### References

1. RA Ford, C Letizia and AM Api, Monographs on fragrance raw materials,  $\alpha,\alpha,\alpha$ -Dimethyl-p-ethylphenylpropanal. *Food and Chemical Toxicology*, 26(4) 307 (1988)
2. H Li and J Shao, Synthesis of seawind aldehyde with phase transfer catalysis. *Huaxue Shijie*, 29(9) 392–394 (1988)
3. Most of the information on organoleptic properties and uses are taken from: PMP 96, *Database of Perfumery Materials & Performance*, Boelens Aroma Chemicals Information Services, Netherlands; some of the organoleptic information and uses is cited from supplier specification sheets, i.e. IFF and Symrise.

**3-(4-Ethylphenyl)-2,2-dimethylpropionaldehyde exists as a main isomer (60–80%) consisting of an *ortho* isomer (15–35%) and *meta* isomers (ca. 5%)** **F-2**



**3-(4-Ethylphenyl)-2,2-dimethylpropionaldehyde is prepared by condensation of 1-chloromethyl-4-ethylbenzene with isobutyraldehyde in the presence of a phase transfer catalyst** **F-3**



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