

Rose ketones

CAS N°:	23696-85-7 23726-93-4 43052-87-5 24720-09-0 23726-94-5 23726-92-3 23726-91-2 57378-68-4 71048-82-3 39872-57-6 70266-48-7 33673-71-1 35087-49-1 35044-68-9	Empirical formula:	C ₁₃ H ₂₀ O
Synonyms:	<p>23696-85-7 (C₁₃H₁₈O) 1-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-2-buten-1-one 2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl) Damascenone, Floriffone</p> <p>23726-93-4 (C₁₃H₁₈O) (E)-1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one trans-1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one β-Damascenone</p> <p>43052-87-5 α-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- α-Damascone, Dihydrofloriffone α</p> <p>24720-09-0 (E)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one trans-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)but-2-en-1-one 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (2E)- trans-α-Damascone</p> <p>23726-94-5 (Z)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one cis-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one 2-Buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (Z)- cis-α-Damascone</p> <p>23726-92-3 1-(2,6,6-Trimethylcyclohex-1-en-1-yl)but-2-en-1-one (Z)-β-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one (Z)-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one 2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (2Z)- cis-β-Damascone, Damasione</p> <p>23726-91-2 (2E)-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one (E)-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one 1-(2,6,6-Trimethylcyclohex-1-en-1-yl)but-2-en-1-one trans-β-Damascone, Dihydrofloriffone β</p>		

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57378-68-4

δ-1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one 2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-

1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one

δ-Damascone, Dihydrofloriffone TD

71048-82-3

[1α(E),2β]-1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one

[1α(E),2β]-1-(2,6,6-Trimethylcyclohex-3-en-1-yl)but-2-en-1-one

trans,trans-δ-Damascone

39872-57-6

1-(2,4,4-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one

(E)-1-(2,4,4-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one

2-Buten-1-one, 1-(2,4,4-trimethyl-2-cyclohexen-1-yl)-, (2E)-

2-Buten-1-one, 1-(2,4,4-trimethyl-2-cyclohexen-1-yl)-, (E)-

Isodamascone (high α)

70266-48-7

1-(2,4,4-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one

2-Buten-1-one, 1-(2,4,4-trimethyl-1-cyclohexene-1-yl)

Isodamascone (standard quality)

33673-71-1

1-(2,4,4-Trimethylcyclohex-2-en-1-yl)but-2-en-1-one

1-(2,4,4-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one

2-Buten-1-one, 1-(2,4,4-trimethyl-2-cyclohexen-1-yl)-

Isodamascone (isomer unspecified)

35087-49-1

1-(2,2-Dimethyl-6-methylenecyclohexyl)but-2-en-1-one

2-Buten-1-one, 1-(2,2-dimethyl-6-methylenecyclohexyl)-

Damascone g-, γ-Damascone

35044-68-9

2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

2,6,6-Trimethyl-1-(2-butenoyl)-1-cyclohexene

2,6,6-Trimethyl-1-crotonoyl-1-cyclohexene

1-(2,6,6-Trimethylcyclohexenyl)-2-buten-1-one

1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one

Damascone b-, β-Damascone

History:	Initial reviews:	December 1991, December 1995, July 2007 (42th Amendment), July 2008 (43th Amendment)	
	Current revision date:	2009	
	Implementation date:	For new submissions*:	August 7, 2009
		For existing fragrance compounds*:	August 7, 2011
Next review date	2014		

* This date applies to the supply of fragrance compounds (formulas) only, not to the finished products in the marketplace.

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RECOMMENDATION:
RESTRICTED

RESTRICTIONS:

Limits in the finished product:

Category 1 See Note box (1)	0.003 %	Category 7	0.008 %
Category 2	0.004 %	Category 8	0.02 %
Category 3	0.02 %	Category 9	0.02 %
Category 4	0.02 %	Category 10	0.02 %
Category 5	0.02 %	Category 11	See Note Box (2)
Category 6	0.07 %		

Note box:

For this material, for pragmatic reasons, restrictive levels allowed by the QRA for certain categories but actually being higher than those already in place before applying the QRA, will temporarily not be implemented until the end of a 5 year monitoring phase. At the end of the 5 years the position will be re-evaluated again.

The above limits apply to Rose Ketones used individually or in combination.

(1) IFRA would recommend that any material used to impart perfume or flavour in products intended for human ingestion should consist of ingredients that are in compliance with appropriate regulations for foods and food flavourings in the countries of planned distribution and, where these are lacking, with the recommendations laid down in the Code of Practice of IOFI (International Organisation of the Flavor Industry) (<http://www.iofiorg.org/>).

(2) Category 11 includes all non-skin contact or incidental skin contact products. Due to the negligible skin contact from these types of products there is no justification for a restriction of the concentration of this fragrance ingredient in the finished product.

Fragrance material specifications:

N/A

CONTRIBUTION FROM OTHER SOURCES:

None to consider (see also the note on contributions from other sources in the **Introduction to the IFRA Standards**).

CRITICAL EFFECT:
SENSITIZATION
RIFM SUMMARIES:

See Enclosures.

REXPAN RATIONALE / CONCLUSION:

The RIFM Expert Panel reviewed the critical effect data for Rose Ketones and, based on the weight of evidence, established the No Expected Sensitization Induction Level (NESIL) as 100 µg/cm². They recommend the limits for the 11 different product categories, which are the acceptable use levels of Rose Ketones in the various product categories. These were derived from the application of the exposure-based quantitative risk assessment approach for fragrance ingredients, which is detailed in the QRA Expert Group Technical Dossier of June 22, 2006.

REFERENCES:
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RIFM (Research Institute for Fragrance Materials, Inc.), 1979a. Evaluation of potential hazards of alpha-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2-buten-1-one by dermal contact in human subjects. Unpublished report from IFF Inc., 17 September. RIFM report number 15397. (RIFM, Woodcliff Lake, NJ, USA).

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trans-alpha-Damascone, (E)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one (24720-09-0)

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cis-beta-Damascone, (Z)-beta-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one (23726-92-3)

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RIFM (Research Institute for Fragrance Materials, Inc.), 1980. Repeat insult patch test with (Z)-beta-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-buten-1-one. Unpublished report from IFF, Inc., 17 June. Report number 47353. (RIFM, Woodcliff Lake, NJ, USA).

trans-beta-Damascone, (2E)-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one (23726-91-2)

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delta-Damascone, delta-1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one (57378-68-4)

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trans,trans-delta-Damascone, [1alpha(E),2beta]-1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one (71048-82-3)

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Isodamascone (standard quality), 1-(2,4,4-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one (70266-48-7)

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gamma-Damascone, 1-(2,2-Dimethyl-6-methylenecyclohexyl)but-2-en-1-one (35087-49-1)

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