ROSE KETONES

CAS Nº: 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: **23696-85-7** ($C_{13}H_{18}O$)
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

23726-93-4 ($C_{13}H_{18}O$)
(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

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

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

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

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

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

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

ROSE KETONES

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.

ROSE KETONES

Standard: RESTRICTED

RESTRICTIONS:

Limits in the finished product:
For a description of the categories, refer to the QRA Information Booklet.

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 - See Note box (1)	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 - 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 specification: 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/cm^2. 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

ROSE KETONES

References:

Damascenone, 1-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-2-buten-1-one (23696-85-7)
RIFM (Research Institute for Fragrance Materials, Inc.), 1978. Repeated insult patch test of 1-(2,6,6-trimethylcyclohexa-1,3-dienyl)-2-buten-1-one in human subjects. RIFM report number 15395, July 12 (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 2001. Murine local lymph node assay with 1-(2,6,6-trimethylcyclohexa-1,3-dienyl)-2-buten-1-one in mice. Unpublished report from Firmenich Incorporated, Report number 38813 (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 2002. 1-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-2-buten-1-one: local lymph node assay in mice. Unpublished report from Firmenich Incorporated, 22 October. Report number 41991 (RIFM, Woodcliff Lake, NJ, USA).
alpha-Damascone, alpha-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one (43052-87-5)
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).
RIFM (Research Institute for Fragrance Materials, Inc.), 1979b. Repeated insult patch test of alpha-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2-buten-1-one in humans. Unpublished report from Firmenich Inc., 19 December. RIFM report number 153414. (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 1985. Maximization study of alpha-1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2-buten-1-one in humans. Unpublished report from Firmenich Inc., 29 July. RIFM report number 15416. (RIFM, Woodcliff Lake, NJ, USA).
trans-alpha–Damascone, (E)-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one (24720-09-0)
RIFM (Research Institute for Fragrance Materials, Inc.), 2001. Murine local lymph node assay with 2-buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (2E)- in mice. Unpublished report from Firmenich Incorporated, Report number 38814 (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 2001a. Repeated insult patch study of 2-buten-1-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (2E)- at 0.5% in diethyl phthalate (DEP). Unpublished report from Firmenich Incorporated, Report number 38815 (RIFM, Woodcliff Lake, NJ, USA).
cis-beta-Damascone, (Z)-ß-1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one (23726-92-3)
RIFM (Research Institute for Fragrance Materials, Inc.), 1979. Repeated insult patch test of beta-damascone in human subjects. Unpublished report from IFF, Inc., 19 February. RIFM report number 15394. (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 1980. Repeat insult patch test with (Z)-b-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)
RIFM (Research Institute for Fragrance Materials, Inc.), 1979. Repeated insult patch test of (2E)-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-buten-1-one in humans. Unpublished report from Firmenich, Inc., 19 December. Report number 15407. (RIFM, Woodcliff Lake, NJ, USA).

ROSE KETONES

RIFM (Research Institute for Fragrance Materials, Inc.), 2001. Murine local lymph node assay with (2E)-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-buten-1-one. Unpublished report from Firmenich, Inc. Report number 38811. (RIFM, Woodcliff Lake, NJ, USA).

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

RIFM (Research Institute for Fragrance Materials, Inc.), 1982. Evaluation of potential irritation and sensitization hazards of delta-damascone by dermal contact in humans. Unpublished report from International Flavors and Fragrances, 17 November. Report number 15399 (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 2002a. Murine local lymph node assay of delta-1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one. Unpublished report from Firmenich Incorporated, 9 July. Report number 41992 (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 2002b. Murine local lymph node assay of delta-1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one. Unpublished report from Firmenich Incorporated, 2 April. Report number 42139 (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 2004. delta-1-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-2-buten-1-one: Local Lymph Node Assay. Unpublished report from International Flavors and Fragrances, 13 December. Report number 47819 (RIFM, Woodcliff Lake, NJ, USA).

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

RIFM (Research Institute for Fragrance Materials, Inc.), 1978. Repeated insult patch test with [1.alpha.(E),2.beta.]-1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-2-buten-1-one. Unpublished report from International Flavors and Fragrance, 11 August. Report number 50614 (RIFM, Woodcliff Lake, NJ, USA).

Isodamascone (high alpha), (E)-1-(2,4,4-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one (39872-57-6)

RIFM (Research Institute for Fragrance Materials, Inc.), 1994. Repeated insult patch test on isodamascone on human subjects. RIFM report number 25751, July 25 (RIFM, Woodcliff Lake, NJ, USA).
RIFM (Research Institute for Fragrance Materials, Inc.), 1995. Repeated insult patch test of isodamascone in human subjects. RIFM report number 25753, June 20 (RIFM, Woodcliff Lake, NJ, USA).

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

RIFM (Research Institute for Fragrance Materials, Inc.), 1985. Repeated insult patch test with isodamascone. RIFM report number 41231, December 22 (RIFM, Woodcliff Lake, NJ, USA).

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

RIFM (Research Institute for Fragrance Materials, Inc.), 2001. Murine local lymph node assay with 2-buten-1-one, 1-(2,2-dimethyl-6-methylenecyclohexyl)- in mice. Unpublished report from Firmenich Inc. RIFM report number 38812. (RIFM, Woodcliff Lake, NJ, USA).