

ROSA – CETONAS (ROSE KETONES)
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CAS N°: (CAS 23696-85-7: C₁₃H₁₈O)

Fórmula empírica: C₁₃H₂₀O

Nome e sinônimos: ROSE KETONES; CETONAS DE ROSAS

23696-85-7	1-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-2-buten-1-one 1-(2,6,6-Trimeticicloexa-1,3-dienil)-2-buten-1-ona, Damascenone Floriffone
43052-87-5	α-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one 1-(2,6,6-Trimetil-2-cicloexen-1-il)- 2-buten-1-ona, α-Damascone Dihydrofloriffone A
24720-09-0	(E)-1-(2,6,6-Trimethyl-2- cyclohexen -1-yl)-2-buten-1-one 1-(2,6,6-Trimetil-2-cicloexen-1-il)-, (2E)- 2-buten-1-one trans-α-Damascone trans-1-(2,6,6-Trimetil-2- cicloexen -1-il)but-2-en-1-ona
23726-94-5	cis-1-(2,6,6-Trimethyl-2- cyclohexen -1-yl)-2-buten-1-one 2-Buten-1-ona, 1-(2,6,6- trimetil -2- cicloexen -1-il)-, (Z)- cis-α-Damascone (Z)-1-(2,6,6-Trimetil-2- cicloexen -1-il)-2-buten-1-ona
23726-92-3	(Z)-β-1-(2,6,6-Trimethyl-1- cyclohexen -1-yl)-2-buten-1-one 2-Buten-1-ona, 1-(2,6,6- trimetil -1- cicloexen -1-il)-, (2Z)- cis-β-Damascone Damasione (Z)-1-(2,6,6-Trimetil-1- cicloexen -1-il)-2-buten-1-ona
23726-91-2	(2E)-1-(2,6,6-Trimethyl-1- cyclohexen -1-yl)-2-buten-1-one trans-β-Damascone Dihydrofloriffone B (E)-1-(2,6,6-Trimetil-1- cicloexen -1-il)-2-buten-1-ona
57378-68-4	δ-1-(2,6,6-Trimethyl-3- cyclohexen -1-yl)-2-buten-1-one 2-Buten-1-ona, 1-(2,6,6- trimetil -3- cicloexen -1-il)- δ-Damascone Dihydrofloriffone TD 1-(2,6,6-Trimetil-3- cicloexen -1-il)-2-buten-1-ona
71048-82-3	[1.α.(E),2.β.]1-(2,6,6-Trimethyl-3- cyclohexen -1-yl)-2-buten-1-one trans,trans-.δ.-Damascone [1.α.(E),2.β.]1-(2,6,6-Trimetilcicloex-3-en-1-il)but-2-en-1-ona
39872-57-6	(E)-1-(2,4,4-Trimethyl-2- cyclohexen -1-yl)-2-buten-1-one 2-Buten-1-ona, 1-(2,4,4-trimetil-2- cicloexen -1-il)-, (2E)- 2-Buten-1-ona, 1-(2,4,4-trimetil-2- cicloexen -1-il)-, (E)- Isodamascone (high α)
70266-48-7	1-(2,4,4-Trimethyl-1- cyclohexen -1-yl)-2-buten-1-one 2-Buten-1-ona, 1-(2,4,4-trimetil-1-cicloexen-1-il) Isodamascone (qualidade standard)

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33673-71-1	1-(2,4,4-Trimethyl-2- cycloexen -1-yl)-2-buten-1- one 2-Buten-1-ona, 1-(2,4,4-trimetil-2- cicloexen -1-il)- Isodamascone (isômero não espeffico)
35087-49-1	1-(2,2-Dimethyl-6-methylenecyclohexil) but-2-en-1-one 2-Buten-1-ona, 1-(2,2-dimetil-6-metilenecicloexil)- γ-Damascone

Histórico:	Revisões anteriores:	Dezembro 1991, Dezembro 1995, Maio 2007 (42° Aditamento)
	Data da revisão atual:	2007
	Data de implementação:	<u>para novas apresentações*</u> : 16/08/2008 <u>para composições de fragrâncias existentes*</u> : 16/08/2010
	Data da próxima revisão:	2013

* Esta data refere-se somente ao fornecimento de composições de fragrâncias (fórmulas), mas não a produtos de consumo existentes no mercado.

NORMA: COM RESTRIÇÕES

RESTRIÇÕES:

Limites no produto final:

A descrição das categorias encontra-se no Livro de Informação sobre a QRA (Quantitative Risk Assessment) – Avaliação Quantitativa de Risco

Categoria 1* ⁽¹⁾	0,003 %	Categoria 7	0,008 %
Categoria 2	0,004 %	Categoria 8	0,02 %
Categoria 3	0,02 %	Categoria 9	0,02 %
Categoria 4	0,02 %	Categoria 10	0,02 %
Categoria 5	0,02 %	Categoria 11	Sem restrições ⁽²⁾
Categoria 6* ⁽¹⁾	0,07 %		

Observações:

Por razões pragmáticas, embora os níveis de restrição permitidos para esta substância pela QRA sejam maiores em certas categorias do que aqueles já implementados antes da aplicação da QRA, eles não serão introduzidos antes que termine o período de monitoramento por 5 anos.

(1) A IFRA recomenda que qualquer material utilizado para conferir perfume ou sabor a produtos de ingestão humana presumível, deve ser constituído por ingredientes que estão em conformidade com as regulamentações pertinentes para alimentos e aromatizantes para alimentos vigentes nos países de distribuição prevista e, na falta destas, devem atender as recomendações do Código de Boas Práticas da IOFI (International Organisation of the Flavor Industry) www.iofiorg.org.

(2) A categoria 11 inclui todos produtos que não têm contato com a pele e aqueles de contato casual. Em vista do contato desprezível deste tipo de produtos, não há justificativa para estabelecer restrição da concentração deste ingrediente de fragrância no produto final.

Especificação da matéria-prima para fragrâncias: não aplicável

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Contribuição de outras fontes: Nenhuma a ser considerada (veja também a observação sobre contribuição de outras fontes na introdução das Normas da IFRA).

Efeito crítico: Sensibilização

Sumário do RIFM: Veja os documentos nas referências

Análise / Conclusão do REXPAN:

O RIFM Expert Panel revisou os dados sobre o efeito crítico de rose ketones e, baseado no peso da evidência estabeleceu o “No Expected Sensitization Induction Level” - NESIL em 24 µg/cm². Recomendou limites para as 11 categorias de produtos, que correspondem às concentrações de uso aceitável do carbonato de metil octino nas várias categorias de produtos. Estes dados foram obtidos através da avaliação quantitativa de risco de ingredientes de fragrâncias em função da exposição ao produto, conforme detalhado no dossiê técnico do QRA Expert Group, de 22 de junho de 2006

Referências:

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).

α-Damascone, α-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-α-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).

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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- β -Damascone, (Z)- β -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- β -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).

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).

 **δ -Damascone, δ -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- δ -Damascone, [1. α .(E),2. β .]-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 α), (E)-1-(2,4,4-Trimethyl-2-cyclohexen-1-yl)-2-buten-1-one
(39872-57-6)**

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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).

γ -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).