

C E T O N E S D E R O S A S
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Fórmula empírica: C₁₃H₂₀O
(CAS 23696-85-7: C₁₃H₁₈O)

CAS Nº:	Nome e sinônimos: CETONAS DE ROSAS
23696-85-7	1-(2,6,6-Trimethylcyclohexa-1,3-dienyl)-2-buten-1-one 1-(2,6,6-Trimetilcicloexa-1,3-dienil)-2-buten-1-ona 2-Buten-1-ona, 1-(2,6,6-trimetil-1,3-cicloexadien-1-il) Damascenone Floriffone
43052-87-5	α-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)- α-Damascone Dihydrofloriffone A
24720-09-0	(E)-1-(2,6,6-Trimethyl-2- cyclohexen -1-yl)-2-buten-1-one 2-Buten-1-one, 1-(2,6,6-trimetil-2-cicloexen-1-il)-, (2E)- trans-α-Damascone trans-1-(2,6,6-Trimetil-2- cicloexen -1-il)but-2-en-1-one
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)

CETONES DE ROSAS

Observações:

Os limites acima aplicam-se a rose ketones utilizadas individualmente ou em combinação.

(1) A IFRA recomenda que, qualquer material utilizado para conferir perfume ou aroma em produtos de ingestão humana deveria ser constituído por ingredientes que estão em conformidade com os regulamentos específicos para alimentos e aromas existentes nos países previstos para sua distribuição e, quando inexistentes, deveriam seguir as recomendações divulgadas no Código de Boas Práticas de Fabricação da IOFI (International Organisation of the Flavor Industry). Informações detalhadas podem ser encontradas no site (www.iofi.org).

(2) A categoria 11 inclui todos produtos sem contato com a pele ou aqueles de contato casual. Em virtude de contato desprezível com a pele, a concentração deste ingrediente de fragrância não deve exceder a concentração usual da composição de fragrância no produto acabado.

Por exemplo, supondo-se que a concentração usual de uma composição no produto final seja de 5% em uma vela perfumada, qualquer ingrediente individual da fragrância (neste caso rose ketones) não deve exceder 5% nesta vela.

Especificação da matéria-prima para fragrâncias: não aplicável

Contribuições 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:

Rose ketones - Estimativa do potencial de sensibilização baseada no peso da evidência

CAS N°	LLNA média ponderada dos valores EC3 (µg/cm ²) [n° de estudos]	Dados em humanos			Potencial Classificação ²	WOE NESIL ³ (µg/cm ²)
		NOEL – HRIPT (indução) (µg/cm ²)	NOEL – MAX (indução) (µg/cm ²)	LOEL ¹ (indução) (µg/cm ²)		
57378-68-4	1579 [3]	NA	NA	1333	Moderado	100 [LLNA weighted mean for class = 1496 µg/cm ²]
43052-87-5	NA	133 (51)	0.2%	NA	Moderado	
24720-09-0	826 [1]	500 (DEP)	NA	NA	Moderado	
23696-85-7	308 [2]	100 (23)	NA	1000	Moderado	
23726-92-3	NA	67 (53)	NA	375	Moderado	
23726-91-2	600	1000 (pet/54)	NA	NA	Moderado	
23726-94-5	NA	NA	NA	NA	Moderado	
39872-57-6	NA	236 (DEP)	NA	2362	Moderado	
71048-82-3	NA	100 (24)	NA	1000	Moderado	
33673-71-1	NA	NA	NA	NA	Moderado	
70266-48-7	NA	1181 (DEP)	NA	NA	Moderado	

CETONES DE ROSAS

NOEL = No observed effect level; concentração/nível sem efeitos observados
HRIPT = Human Repeat Insult Patch Test; teste de contato repetitivo em humanos
MAX = Human Maximization Test; teste de maximização em humanos
LOEL = Lowest observed effect level; concentração/nível de menor efeito observado
NA = Not Available; não disponível

¹Dados obtidos no HRIPT ou no MAX

²Gerberick *et al.*, 2001

³WoE NESIL limitado a dois dados significativos

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 100 µg/cm². Recomendou limites para as 11 categorias de produtos, os quais correspondem às concentrações de uso aceitável de rose ketones nas várias categorias de produtos. Estes dados foram obtidos através da aplicação do método quantitativo de avaliação de risco de ingredientes de cosméticos em função da exposição ao produto, o qual foi detalhado do 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).

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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).

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).

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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)

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).