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Volume 36

Allyl Compounds, Aldehydes, Epoxides and Peroxides

Summary of Data Reported and Evaluation

Allyl compounds

[Allyl chloride](#)
[Allyl isothiocyanate](#)
[Allyl isovalerate](#)
[Eugenol](#)

Aldehydes

Acetaldehyde
Malonaldehyde

Epoxide

[Diglycidyl resorcinol ether](#)

Peroxides

Benzoyl peroxide
Hydrogen peroxide
[Lauroyl peroxide](#)

Last updated: 13 April 1999

ALLYL CHLORIDE

VOL.: 36 (1985) (p. 39)

CAS No.: 107-05-1

Chem. Abstr. Name: 1-Propene, 3-chloro-

5. Summary of Data Reported and Evaluation

5.1 Exposure data

Allyl chloride has been produced commercially since 1945 and is used almost exclusively as a chemical intermediate, principally in the production of epichlorohydrin.

5.2 Experimental data

Allyl chloride has been tested for carcinogenicity by intragastric intubation in mice and rats, by skin application in mice, both by repeated application and in a two-stage assay, and by intraperitoneal injection in mice. Following its oral administration to mice, a nonsignificant increase in the incidence of squamous-cell papillomas and carcinomas of the forestomach was observed; the experiment in rats was inadequate for evaluation. No skin tumour was observed in mice following repeated skin applications; however, a single application followed by treatment with 12-*O*-tetradecanoylphorbol 13-acetate gave some evidence that allyl chloride acts as an initiator. Following its intraperitoneal injection to strain A mice, a slight increase in the incidence of lung adenomas was observed.

Inhalation exposure to allyl chloride of high purity did not induce teratogenicity in rats or rabbits.

Allyl chloride caused DNA damage in bacteria, and was mutagenic to bacteria and fungi.

5.3 Human data

No case report or epidemiological study of the carcinogenicity of allyl chloride to humans was available to the Working Group.

5.4 Evaluation

There is *inadequate evidence* for the carcinogenicity of allyl chloride in experimental animals.

In the absence of epidemiological data, no evaluation could be made of the carcinogenicity of allyl chloride to humans.

For definition of the italicized terms, see [Preamble Evaluation](#).

Subsequent evaluation: [Vol. 71 \(1999\)](#)

Synonyms

- AC
- Chlorallylene
- Chloroallylene

- 1-Chloropropene-2
- 3-Chloropropene-1
- 1-Chloro-2-propene
- 3-Chloro-1-propene
- α -Chloropropylene
- 3-Chloropropylene
- 3-Chloro-1-propylene
- NCI-C04615
- 2-Propenyl chloride

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ALLYL ISOTHIOCYANATE

VOL.:36 (1985) (p. 55)

CAS No.: 57-06-7

Chem. Abstr. Name: 1-Propene, 3-isothiocyanato-

5. Summary of Data Reported and Evaluation

5.1 Exposure data

Allyl isothiocyanate occurs widely in natural products in the glucoside sinigrin. Synthetic allyl isothiocyanate has been produced commercially since 1937. Allyl isothiocyanate is also prepared from the seeds of mustard plants, *Brassica nigra* and *B. juncea*. It is used principally as a flavouring agent in a variety of foods. Exposures can also occur from its use as an alcohol denaturant and in external analgesic products.

5.2 Experimental data

Allyl isothiocyanate was tested for carcinogenicity by gastric intubation in mice of one strain and in rats of one strain. In mice, no increase in the incidence of tumours was observed. An increased incidence of epithelial hyperplasia and transitional-cell papillomas of the urinary bladder was observed in male rats only, and some subcutaneous fibrosarcomas occurred in female rats given the high dose.

Allyl isothiocyanate was not teratogenic to mice, rats, hamsters or rabbits, but resorptions were seen in mice and rats.

Allyl isothiocyanate did not induce DNA damage in bacteria. It induced mutations in bacteria and insects and chromosomal aberrations in plants. It did not induce dominant lethal mutations in mice.

5.3 Human data

No case report or epidemiological study of the carcinogenicity of allyl isothiocyanate to humans was available to the Working Group.

5.4 Evaluation

There is *limited evidence* for the carcinogenicity of allyl isothiocyanate to experimental animals.

In the absence of epidemiological data, no evaluation could be made of the carcinogenicity of allyl isothiocyanate to humans.

For definition of the italicized terms, see [Preamble Evaluation](#).

Subsequent evaluations: Suppl. 7 (1987) (p. 56); [Vol. 73 \(1999\)](#)

Synonyms

- AITC
- AITK
- Allyl isorhodanide

- Allyl isosulphocyanate
- Allyl isothiocyanate
- Allyl mustard oil
- Allylsenevol
- Allylsenfol
- Allyl sevenolum
- Allyl thiocarbonimide
- Artificial mustard oil
- Artificial oil of mustard
- Carbospol
- FEMA No. 2034
- 3-Isothiocyanatopropene
- 3-Isothiocyanato-1-propene
- Isothiocyanic acid allyl ester
- NCI-C50464
- Oil of Mustard BPC 1949, Synthetic
- Oleum sinapis
- Oleum sinapis volatile
- 2-Propenyl isothiocyanate
- Propylene-3-isothiocyanate
- Redskin
- Synthetic mustard oil
- Synthetic mustard oil volatile
- Volatile mustard oil
- Volatile oil of mustard

Last updated: 30 September 1999

ALLYL ISOVALERATE

VOL.: 36 (1985) (p. 69)

CAS No.: 2835-39-4

Chem. Abstr. Name: Butanoic acid, 3-methyl-, 2-propenyl ester

5. Summary of Data Reported and Evaluation

5.1 Exposure data

Allyl isovalerate has been used since the 1950s as a fragrance raw material in cosmetics, lotions and perfumes and in certain food products, although it is not known whether it is used in these applications currently.

5.2 Experimental data

Allyl isovalerate was tested for carcinogenicity by intragastric intubation in mice of one strain and in rats of one strain. In mice, it induced papillomas of the forestomach in males and increased the incidence of lymphomas in females. In rats an increased incidence of mononuclear-cell leukaemia was observed in animals of both sexes.

Allyl isovalerate was not mutagenic to bacteria.

5.3 Human data

No case report or epidemiological study of the carcinogenicity of allyl isovalerate to humans was available to the Working Group.

5.4 Evaluation

There is *limited evidence* for the carcinogenicity of allyl isovalerate to experimental animals.

In the absence of epidemiological data, no evaluation could be made of the carcinogenicity of allyl isovalerate to humans.

For definition of the italicized terms, see [Preamble Evaluation](#).

Subsequent evaluation: [Vol. 71 \(1999\)](#)

Synonyms

- Allyl isovalerianate
 - Allyl 3-methylbutyrate
 - FEMA No. 2045
 - Isovaleric acid, allyl ester
 - 3-Methylbutanoic acid, 2-propenyl ester
 - 3-Methylbutyric acid, allyl ester
 - 2-Propenyl isovalerate
 - 2-Propenyl 3-methylbutanoate
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Last updated: 13 April 1999

EUGENOL

VOL.: 36 (1985) (p. 75)

CAS No.: 97-53-0

Chem. Abstr. Name: Phenol, 2-methoxy-4-(2-propenyl)-

5. Summary of Data Reported and Evaluation

5.1 Exposure data

Eugenol occurs widely as a component of essential oils and is a major constituent of clove oil. It has been used since at least the nineteenth century, primarily as a flavouring agent, in a variety of foods and pharmaceutical products, and as an analgesic in dental materials.

5.2 Experimental data

Eugenol was tested in mice of one strain and in rats of one strain by oral administration of a diet containing a high dose of eugenol. In mice, there was a significant increase in the incidence of liver tumours in females; in males, the increase was significant only for those receiving the lower dose. In rats, no increased incidence of tumours was observed. Other studies in mice by oral administration, skin application and intraperitoneal injection were inadequate for an evaluation of carcinogenicity, mainly due to the short duration of treatment.

Eugenol gave both positive and negative results in tests for DNA damage in bacteria. It was not mutagenic in several studies in bacteria. The compound was not active in a host-mediated assay in mice, nor was the urine of rats treated with eugenol mutagenic. Eugenol induced chromosomal aberrations and a small increase in sister chromatid exchanges in mammalian cells *in vitro*.

In one two-stage mouse-skin assay, 2',3'-epoxyeugenol, an in-vitro metabolite of eugenol, showed initiating activity.

2',3'-Epoxyeugenol was mutagenic to bacteria. Two urinary metabolites of eugenol, 3-piperidyl-1-(3'-methoxy-4'-hydroxyphenyl)-1-propanone and 3-pyrrolidinyl-1-(3'-methoxy-4'-hydroxyphenyl)-1-propanone were not mutagenic to bacteria or in the host-mediated assay.

5.3 Human data

No case report or epidemiological study of the carcinogenicity of eugenol to humans was available to the Working Group.

5.4 Evaluation

There is *limited evidence* for the carcinogenicity of eugenol to experimental animals.

In the absence of epidemiological data, no evaluation could be made of the carcinogenicity of eugenol to humans.

For definition of the italicized terms, see [Preamble Evaluation](#).

Subsequent evaluation: Suppl. 7 (1987) (p. 63: **Group 3**)

Synonyms

- 4-Allylcatechol-2-methyl ether
- Allylguaiacol
- 4-Allylguaiacol
- *para*-Allylguaiacol
- 1-Allyl-4-hydroxy-3-methoxybenzene
- 4-Allyl-1-hydroxy-2-methoxybenzene
- Caryophyllic acid
- Eugenol
- 1,3,4-Eugenol
- *para*-Eugenol
- FEMA No. 2467
- 1-Hydroxy-4-allyl-2-methoxybenzene
- 4-Hydroxy-3-methoxyallylbenzene
- 1-Hydroxy-2-methoxy-4-allylbenzene
- 1-Hydroxy-2-methoxy-4-propenylbenzene
- 1-Hydroxy-2-methoxy-4-prop-2-enylbenzene
- 2-Methoxy-4-allylphenol
- 2-Methoxy-1-hydroxy-4-allylbenzene
- 2-Methoxy-4-prop-2-enylphenol
- 2-Methoxy-4-(2-propenyl)phenol
- 2-Methoxy-4-(2-propen-1-yl)phenol
- NCI-C50453

Last updated: 20 April 1998

DIGLYCIDYL RESORCINOL ETHER

VOL.: 36 (1985) (p. 181)

CAS No.: 101-90-6

Chem. Abstr. Name: Oxirane, 2,2'-[1,3-phenylenebis(oxyethylene)]bis-

5. Summary of Data Reported and Evaluation

5.1 Exposure data

Diglycidyl resorcinol ether has been produced since at least 1974. It has only limited application, principally in the aerospace industry.

5.2 Experimental data

Diglycidyl resorcinol ether (of technical grade) was tested for carcinogenicity by intragastric intubation in mice of one strain and in rats of one strain. It induced squamous-cell carcinomas and papillomas of the forestomach in animals of both species. In female mice, an increased incidence of hepatocellular tumours was observed. In one experiment in mice, no skin tumour was observed after skin application.

Diglycidyl resorcinol ether (of technical grade) was mutagenic to bacteria.

5.3 Human data

No case report or epidemiological study of the carcinogenicity of diglycidyl resorcinol ether to humans was available to the Working Group.

5.4 Evaluation

There is *sufficient evidence* for the carcinogenicity of a technical grade of diglycidyl resorcinol ether to experimental animals.

No data on the carcinogenicity of diglycidyl resorcinol ether to humans were available to the Working Group.

For definition of the italicized terms, see [Preamble Evaluation](#).

Previous evaluation: [Vol. 11 \(1976\)](#)

Subsequent evaluation: [Vol. 71 \(1999\)](#)

Synonyms

- Araldite ERE 1359
- 1,3-Bis(2,3-epoxypropoxy)benzene
- *meta*-Bis(glycidyl)benzene
- Diglycidyl ether of resorcinol
- 1,3-Diglycidylbenzene
- Diglycidyl resorcinol
- NCI-C54966

- 2,2'-[1,3-Phenylenebis(oxymethylene)]bisoxirane
- RDGE
- Resorcinol bis(2,3-epoxypropyl)ether
- Resorcinol diglycidyl ether
- Resorcinol glycidyl ether
- Resorcinyldiglycidyl ether

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LAUROYL PEROXIDE

VOL.: 36 (1985) (p. 315)

CAS No.: 105-74-8

5. Summary of Data Reported and Evaluation

5.1 Exposure data

Lauroyl peroxide was first produced commercially in about 1941. It is used principally in the production of polymers; small amounts are employed in food packaging.

5.2 Experimental data

Lauroyl peroxide was tested by subcutaneous administration in mice and rats and by skin application in mice. In one study in mice by subcutaneous administration, the evidence concerning a carcinogenic effect was inconclusive; in two other studies, no increase in tumour incidence was observed. Two studies in mice by skin application were inadequate for an evaluation of complete carcinogenicity; one study indicated that lauroyl peroxide has promoting activity in mouse skin.

The available data are inadequate to evaluate the teratogenic potential of lauroyl peroxide in mammals.

The available data are inadequate to evaluate the activity in short-term tests of lauroyl peroxide.

5.3 Human data

No case report or epidemiological study of the carcinogenicity of lauroyl peroxide to humans was available to the Working Group.

5.4 Evaluation

There is *inadequate evidence* for the carcinogenicity of lauroyl peroxide to experimental animals.

In the absence of epidemiological data, no evaluation could be made of the carcinogenicity of lauroyl peroxide to humans.

For definition of the italicized terms, see [Preamble Evaluation](#).

Subsequent evaluation: [Vol. 71 \(1999\)](#)

Synonyms

- Alperox C, C/S,F and S-35
- Dilauroyl peroxide
- Dodecanoyl peroxide
- DYP-97F
- Laurox Q and W40
- Laurydol
- LYP 97 and 97F

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