Ethyl heptanoate

Botanical Source

Synonyms HEPTANOIC ACID, ETHYL ESTER; ETHYL HEPTONATE; ETHYL HEPTYLATE; ETHYL n-HEPTOATE; ETHYL HEPTOATE; ETHYL CAPRATE

IUPAC Name ETHYL HEPTANOATE

CAS Reference 106-30-9

E Number

Food Legislation

Council of Europe (CoE)	
Number	Comment
365	Listed by the Council of Europe as acceptable for use in food.

US Food and Drug Administration	
Number	Comment
172.515	Approved by the US FDA. FDA 21 CFR 172.515

Joint FAO/WHO Expert Committee on Food Additives (JECFA)		
Number	ADI	Comment
32	220	ADI 0-2.5 mg/kg bw

FEMA	
FEMA No.	Comment
2437	Generally recognised as safe as a flavour ingredient:GRAS List Number 3

Natural Occurrence and Use in Food
Found in cashew apple, cocoa, grape, grapefruit juice, hazelnut roasted, hops, milk, olive, papaya mountain, passion fruit, peach; used in chewing gum.

Estimated Intake from Food and Drink	
Daily Intake mg/kg/day	FEMA Possible Average Daily Intake mg

0.003149	6.734

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Tobacco Product Related Chemical and Biological Studies for Ingredients Added in a Mixture

Smoke Chemistry		
Published Source	Level Tested %	Comment
BAT	0.00550	At maximum application level this ingredient is not associated with significant increases in levels of Hoffmann analytes in smoke.
Philip Morris	0.01040	An overall assessment of the data suggests that this ingredient did not add to the toxicity of smoke.

Ames Activity		
Published Source	Level Tested %	Comment
BAT	0.00550	Within the sensitivity and specificity of the system the Ames activity of the cigarette smoke condensate was not increased by the addition of the ingredient.
Philip Morris	0.01040	Within the sensitivity and specificity of the system the Ames activity of the cigarette smoke was not increased by the addition of the ingredient.

Micronucleus		
Published Source	Level Tested %	Comment
BAT	0.00550	Within the sensitivity of the in vitro micronucleus assay the activity of the cigarette smoke condensate was not increased by the addition of the ingredient.

Neutral Red		
Published Source	Level Tested %	Comment
BAT	0.00550	Within the sensitivity of the test system the in vitro cytotoxicity of the cigarette smoke condensate was not increased by the addition of the ingredient.
Philip Morris	0.01040	Within the sensitivity of the test system the in vitro cytotoxicity of the cigarette smoke was not increased by the addition of the ingredient.

Inhalation		
Published Source	Level Tested %	Comment
BAT	0.00550	The results indicate that the addition of the ingredient had no discernible effect on the inhalation toxicity of mainstream smoke.
Philip Morris	0.01040	The data indicate that the addition of the ingredient, when added with one of three groups, did not increase the inhalation toxicity of the smoke.

Mouse Skin Painting		
Published Source	Level Tested %	Comment

References

Baker RR, Pereira da Silva JR, Smith G. The effect of tobacco ingredients on smoke chemistry. Part I: Flavourings and additives. Food Chem Toxicol. 2004; 42 Suppl:S3-37.

Baker RR, Pereira da Silva JR, Smith G. The effect of tobacco ingredients on smoke chemistry. Part II: casing ingredients. Food Chem Toxicol. 2004; 42 Suppl:S39-52.

Baker RR, Massey ED, Smith G. An overview of the effects of tobacco ingredients on smoke chemistry and toxicity. Food Chem Toxicol. 2004; 42 Suppl:S53-83.

Carmines EL. Evaluation of the potential effects of ingredients added to cigarettes. Part 1: cigarette design, testing approach, and review of results. Food Chem Toxicol. 2002; 40(1): 77-91.

Rustemeier K, Stabbert R, Haussmann HJ, Roemer E, Carmines EL. Evaluation of the potential effects of ingredients added to cigarettes. Part 2: chemical composition of mainstream smoke. Food Chem Toxicol. 2002; 40(1): 93-104.

Roemer E, Tewes FJ, Meisgen TJ, Veltel DJ, Carmines EL. Evaluation of the potential effects of ingredients added to cigarettes. Part 3: in vitro genotoxicity and cytotoxicity. Food Chem Toxicol. 2002; 40(1): 105-111.

Vanscheeuwijck PM, Teredesai A, Terpstra PM, Verbeeck J, Kuhl P, Gerstenberg B, Gebel S, Carmines EL. Evaluation of the potential effects of ingredients added to cigarettes. Part 4: subchronic inhalation toxicity. Food Chem Toxicol. 2002; 40(1): 113-131.

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Tobacco Product Related Chemical and Biological Studies for Ingredients Tested Singly

References
Baker RR, Bishop LJ. The pyrolysis of tobacco ingredients. J. Anal. Appl. Pyrolysis 2004, 71, 223-311.

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Toxicological Data on the Unburnt Ingredient

[+ve, positive; -ve, negative; ?, equivocal; with, with metabolic activation; without, without metabolic activation]

In vitro

Test system	Test conditions	Endpoint	Activation	Result	References
Salmonella typhimurium, TA97, TA102	Tested up to 1 mg/plate in a preincubation assay	Mutation	with and without S9	-ve (limited assay as only two strains tested)	Fujita & Sasaki, 1987
Bacillus subtilis strains H17 (rec+) and M45 (rec-)	Tested at up to 17 µg/disc, a concentration that was not toxic to either strain (and therefore it was not possible to determine whether there was differential toxicity)	DNA damage (indicated by differential toxicity)	without	No test (reported as -ve, but is in fact a "no test"	Oda *et al* 1978
Bacillus subtilis strains H17 (rec+) and M45 (rec-)	Up to 20 µL/disc, which did not induce toxicity in either strain (and therefore it was not possible to determine whether there was differential toxicity)	DNA damage (indicated by differential toxicity)	without?	No test (as toxicity was not seen in either strain)	Yoo, 1986

References

Fujita H & Sasaki M (1987). Mutagenicity test of food additives with Salmonella

typhimurium TA 97 and TA 102 (II). Tokyo Toritsu Eisei Kenkyusho Nempo, 38, 423-430 (cited in CCRIS, 2003)

Oda Y *et al* (1978). Mutagenicity of food flavours in bacteria (1st report). Osaka-Furitsu Koshu Eisei Kenkyu Hokoku Shokuhin Eisei Hen, 9, 177-181.

Yoo Y S (1986). Mutagenic and antimutagenic activities of flavoring agents used in foodstuffs. J. Osaka City Med. Center, 34, 267-288.