OCTANOIC ACID

New specifications prepared at 63rd JECFA (2004) and published in FNP 52 Add 12 (2004). Small residues of octanoic acid on food (which has been treated with antimicrobial washing solutions) at the time of consumption would not pose a safety concern (63rd JECFA, 2004).

SYNONYMS Caprylic acid

DEFINITION Octanoic acid is manufactured from vegetable oils (coconut, palm, kernel, or palm stearene) by first refining the oil, followed by methyl transesterification and separation by distillation. The separated methyl octanoate is saponified and acidified to give octanoic acid.

Chemical name	Octanoic acid
C.A.S. number	124-07-2
Chemical formula	$CH_3(CH_2)_6CO_2H$
Formula weight	144.21
Assay	Not less than 95%

DESCRIPTION Colourless oily liquid having a slight unpleasant odour

FUNCTIONAL USES Antifoaming agent, surfactant. (Material for use as a flavouring agent is specified in FNP 52 Add 5, JECFA No. 99).

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4)	Slightly soluble in water; soluble in most organic solvents
Infrared spectrum (Vol. 4)	The infrared spectrum of a potassium bromide dispersion of the sample corresponds to the reference infrared spectrum in the Annex.
Acid value (Vol. 4)	Between 366 and 396

PURITY

Water (Vol. 4)	Not more than 0.4% (Karl Fischer Method)
Sulfated ash (Vol. 4)	Not more than 0.1% Test 10 g of the sample (Method II)
Unsaponifiable matter	Not more than 0.2% See description under TESTS
Iodine value (Vol. 4)	Not more than 2.0
Decanoic acid	Not more than 3% See description under METHOD OF ASSAY
Lead (Vol. 4)	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the

specified level. The selection of the sample size and method of sample preparation may be based on the principles of the method described in Volume 4, “Instrumental methods”

TESTS

PURITY TESTS

Unsaponifiable matter

Weigh accurately 5.0 g of the sample into a 250 ml flask, add a solution of 2 g of potassium hydroxide in 40 ml of alcohol, and boil gently under a reflux condenser for 1 h or until saponification is complete. Transfer the contents of the flask to a glass-stoppered graduated extraction cylinder. Wash the flask with sufficient alcohol to make a volume of 40 ml in the cylinder, and complete the transfer with warm and then cold water until the total volume is 80 ml. Finally, wash the flask with a few ml of petroleum ether, add the washings to the cylinder, cool the contents of the cylinder to room temperature, and add 50 ml of petroleum ether.

Insert the stopper, shake the cylinder vigorously for at least 1 min, and allow both layers to become clear. Siphon the upper layer as completely as possible without removing any of the lower layer, collecting the ether fraction in a 500-ml separator. Repeat the extraction and siphoning at least six times with 50-ml portions of petroleum ether, shaking vigorously each time. Wash the combined extracts, with vigorous shaking, with 25-ml portions of 10% alcohol until the wash water is neutral to phenolphthalein, and discard the washings. Transfer the ether extract to a tared beaker, and rinse the separator with 10 ml of ether, adding the rinsings to the beaker. Evaporate the ether on a steam bath just to dryness, and dry the residue to constant weight, preferably at 75° to 80° under a vacuum of not more than 200 mm of Hg, or at 100° for 30 min. Cool in a desiccator, and weigh to obtain the uncorrected weight of unsaponifiable matter.

Determine the quantity of fatty acids in the residue as follows: Dissolve the residue in 50 ml of warm alcohol (containing phenolphthalein TS and previously neutralized with sodium hydroxide to a faint pink colour), and titrate with 0.02 N sodium hydroxide to the same colour. Each ml of 0.02 N sodium hydroxide is equivalent to 5.659 mg of fatty acids, calculated as oleic acid.

Subtract the calculate weight of fatty acids from the weight of the residue to obtain the corrected weight of unsaponifiable matter in the sample.

METHOD OF ASSAY

Determine using an appropriate gas chromatographic technique. The selection of sample size and method of sample preparation may be based on AOCS Method Cc 1-62 and Ce 1f-96 and follow the principles of the method described in FNP 5 "Instrumental methods". The percentage of octanoic acid is the area percent of the methyl octanoate peak.

Decanoic acid may be determined using the same gas chromatographic technique.