

#### **COVID-19 Information**



Public health information (CDC) Research information (NIH) SARS-CoV-2 data (NCBI) Prevention and treatment information (HHS) Español



DATA SOURCES > HAZARDOUS SUBSTANCES DATA BANK (HSDB) > ANNOTATION RECORD

# NONANOIC ACID

**Hazardous Substances** 5554 **DataBank Number** Related CIDs **Related PubChem Records** 

8158

### 1 Human Health Effects



# 1.1 Human Toxicity Excerpts (Complete)



/HUMAN EXPOSURE STUDIES/ A 12% soln of nonanoic acid in petrolatum produced no irritation on human skin after a 48-hr closed patch test. ... no sensitization reactions were produced in 25 volunteers after patch testing with nonanoic acid (12% in petrolatum).

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 735

/HUMAN EXPOSURE STUDIES/ Various concn of nonanoic acid in 1-propanol were applied to 116 healthy volunteers and 75 dermatitis patients as a positive control for patch testing. A dose of 20% produced skin reactions in 90.1-93.9% of subjects. Lesions consisted of erythema at 48 hr & pigmentation @ 96 hr.

#### PMID:7398264

WAHLBERG JE, MAIBACH HI; CONTACT DERMATITIS 6 (2): 128 (1980)

/HUMAN EXPOSURE STUDIES/ ... (0.5 OR 1.0 Molar in propanol) caused irritation /in humans/ when applied under occlusive patches.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3559

/HUMAN EXPOSURE STUDIES/ Skin reactions to 40% nonanoic acid in propanol (NON) ... were evaluated by image analysis of 20 MHz B scan recordings (Dermascan C, Cortex Technology). 18 women, aged 18 to 45, were patch tested with 24-hr application time, and clinical and instrumental evaluations were performed at the beginning of the experiment, and 24 and 48 hr after patch testing. To check possible regional variations ... /NON/ was applied 2 x on the same forearm. As control tests, saline solution, propanol and sodium lauryl sulfate (SLS) 3% were applied. Echographic images were processed by a program enabling numerical representation of picture data, based on attribution of fictional values to the echoes' amplitudes, selection of amplitude bands of interest, binary transformation of the image, and calculation of the extension of areas reflecting within the same amplitude range. Sonographic recordings were evaluated by an amplitude interval marking hyporeflecting parts of the dermis (corresponding to edema and inflammatory infiltration), and by a band highlighting the entrance echo (epidermis) ... Evaluations showed that extension of the hypoechogenic area of the dermis increases according to intensity of inflammatory reaction for all irritant substances. A clear decrease in reflectivity of the epidermis echo at 24 hr was

visible at SLS patch test sites, whereas at patch test sites performed with NON ... there was a trend towards an increase in values of hyperreflecting pixels. No significant variations between data recorded at proximal compared to distal skin sites were observed ... /40% Nonanoic acid in propanol/

#### PMID:7821005

Seidenari S; Contact Dermatitis 31(3):146-50 (1994)

/HUMAN EXPOSURE STUDIES/ Variable types of skin irritation were induced in 8 human female volunteers, ranging from subclinical to visible erythema with slight edema. Skin reactions were graded clinically and objectively using transepidermal water loss (TEWL), laser Doppler flowmetry (LDF) and improved reflectance spectroscopy. This last technique enables separation of in vivo erythemas into relatively deoxygenated (venous--deoxy hem) and oxygenated (arterial--oxy hem) hemoglobin components. Compared to uninvolved skin, an empty patch increased oxy hem by 197% + / - 121% (p < 0.05). Exposure to vehicles also changes skin biophysics ... Nonanoic acid (NON) ... raised oxy hem, LDF and TEWL values linearly at increasing concentrations ... The improved reflectance spectroscopic technique proved valid in skin irritation studies, with a higher sensitivity than laser Doppler flowmetry, and allowed irritant vascular reactions to be discriminated into arterial and venous components ...

#### PMID:8565486

Andersen PH, Maibach HI; Contact Dermatitis 33(5):315-22 (1995)

/HUMAN EXPOSURE STUDIES/ In this study of 152 women, comparison of patch test responses between 2 irritants over 96 hr at 2 symmetrical anatomical sites is studied. 2 irritants, each at 4 different concentrations (nonanoic acid (NAA) 80%, 40%, 20%, 10%; sodium lauryl sulfate (SLS) 3%, 2%, 1% and 0.5%) and using propan-1ol and 'water for injection' as the respective controls, were placed as 15 uL aliquots, soaked onto filter paper discs in Finn Chambers, on the volunteer's left and right lower back. The patches were removed at 47, and read at 48 and 96 hr. Irritant reactions were evaluated for erythema and surface changes by degree and area affected. Statistical analysis of the results showed that erythema decreased with time for all concentrations of NAA, and at higher concentrations for SLS. Surface changes increased with time for SLS and at higher concentrations of NAA. There was no statistically significant difference comparing left and right sides. Traditionally in patch testing, reactions which fade after 48 hr have been regarded as irritant rather than allergic. This study refutes that assumption. Data from ... left to right comparisons, made in the same individuals at the same time, show that irritant reactions may be more reproducible than previously appreciated.

#### PMID:9840260

Reiche L et al; Contact Dermatitis 39(5):240-3 (1998)

/HUMAN EXPOSURE STUDIES/ Keratinocyte proliferation in normal human skin was induced by ... nonanoic acid (NAA) ... at three different concentrations to normal human skin in vivo under occlusion for 24 hr. The irritative response was visually assessed for erythema, and the number of cycling cells was calculated from the number of Ki67 positive cells in cryosections from skin biopsies taken at 0, 24, 48, 72 and 96 hr. In addition, to determine the elemental content of the epidermal cells during the response, two epidermal strata were examined by X-ray microanalysis (XRMA) ... Application of ... NAA resulted in erythema, and the number of Ki67 positive cells was increased at 48 hr. XRMA revealed an initial increase in the sodium/potassium (Na/K) ratio, indicating cell membrane injury. Due to an increasing potassium (K) concentration the Na/K ratio decreased after 24 hr, which is compatible with proliferation, in accordance with the Ki67 data ... The effects of NAA ... /may cause/ proliferation /taking/ place in parallel with cell damage.

#### PMID:10877100

Grangsjo A et al; J Submicrosc Cytol Pathol 32(1):11-6 (2000)

/HUMAN EXPOSURE STUDIES/ Twelve subjects were tested on the forearms using 24 hr occlusive application of three concentrations of ... nonanoic acid (NON) ... Cutaneous blood flow at baseline, the increase in cutaneous blood flow and the skin area having increased perfusion were measured on day 2, day 3 and day 5 ... The area with increased perfusion exceeded the area with clinically visible skin reactions for irritant reactions of grade 1/2 and above ... A correlation was found between clinical scores ... and the mean flow and the area with increased flow ...

#### PMID:12005117

Fullerton A et al; Skin Res Technol 8(1):23-31 (2002)

/HUMAN EXPOSURE STUDIES/ ... Irritant reactions to ... nonanoic acid (NAA) (40%) /were evaluated/ ... The patch

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test responses /to nonanoic acid (NAA) (40%)/ in 40 healthy male and female volunteers between 20 and 30 years of age (20 in each laboratory) /were studied/ with an instrument for measuring skin electrical impedance (IMP). 2 other bioengineering methods and visual scoring were also used to facilitate further illumination of any findings ...

PMID:14641117

Kuzmina N et al; Contact Dermatitis 49(1):26-31 (2003)

/HUMAN EXPOSURE STUDIES/ ... A test procedure which acts as a model for compromised skin and which reproduces on the target sites the cumulative insult which results from repeated exposure, working temperatures, hydration and the action of surfactants /was described/ ... Forearm skin /was immersed/ in an aqueous solution of sodium dodecyl sulfate until an identifiable alteration of skin condition is produced ... The influence of skin compromise on the response to ... nonanoic acid, has been assessed ... /Nonanoic acid/ produced a greater degree of reaction on skin compromised to be within the normal clinical range one might expect from housework.

PMID:8458223

Allenby CF et al; Contact Dermatitis 28(2):84-8 (1993)

/ALTERNATIVE and IN VITRO TESTS/ Exposure to irritants may cause chronic irritant contact dermatitis (ICD),

characterized by irregular epidermal thickening and a predominantly dermal mononuclear cell infiltrate. ... This study examined Langerhans cell (LC) density in clinically normal skin of 46 patients with chronic ICD and 10 healthy individuals, and compared the action of the two irritants nonanoic acid (NA) and sodium lauryl sulfate (SLS) on the LCs and keratinocytes of clinically normal skin in patients with chronic ICD. There was a higher number of LCs/mm basement membrane in patients compared with controls, although there was no difference in the number of dendrites/LC nor in dendrite length. SLS induced keratinocyte proliferation after 48 hr exposure, had no effect on LC number or distribution, and induced keratinocyte apoptosis after 24 and 48 hr exposure. In contrast, NA decreased keratinocyte proliferation after 24 hr exposure but this returned to basal levels after 48 hr, and induced epidermal cell apoptosis after only 6 hr exposure. NA dramatically decreased LC number after 24 and 48 hr exposure, which was accompanied by basal redistribution and decreased dendrite length. Most significantly, NA induced apoptosis in over half of the LCs present after 24 and 48 hr exposure.

PMID:9767290

Forsey RJ et al; Br J Dermatol 139 (3): 453-61 (1998)

/IMMUNOTOXICITY/ Normal human skin was exposed to ... nonanoic acid in isopropanol at different concentrations. The detergents were applied under occlusion in epicutaneous tests for 24 hr and biopsies were taken at 24 or 48 hr. Frozen sections were labelled with monoclonal antibodies against CD1a, CD3 and ICAM-1. The evaluation of the labelled sections showed that there were differential effects on the expression of ICAM-1 and CD1a+ cells in epidermis. After nonanoic acid application ICAM-reactivity could not be detected and there was a decrease of staining for CD1a after exposure to 80% nonanoic acid ... ICAM-1 expression was also detected in normal epidermis in 3 of 9 unexposed control biopsies and after occlusion with ... isopropanol. An increased amount of CD3+ cells was found ...

PMID:1684465

Lindberg M et al; Acta Derm Venereol 71(5): 384-8 (1991)

/OTHER TOXICITY INFORMATION/ ... In 1980, it was suggested that nonanoic acid (NNA) could be used as a positive control when patch testing. Since then, NNA has been used as an experimental irritant in several studies and has been used as a chemically different substance compared to sodium lauryl sulfate (SLS) ...

PMID:14678207

Wahlberg JE, Lindberg M; Contact Dermatitis 49(3):117-23 (2003)

# 1.2 Skin, Eye, and Respiratory Irritations



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Pelargonic acid is a skin and eye irritant.

USEPA; Biopesticide Active Ingredient Fact Sheets - Pelargonic Acid (217500) Fact Sheet (November 6th, 2007). Available from, as of January 18, 2008: http://www.epa.gov/oppbppd1/biopesticides/ingredients/index.htm

Causes substantial but temporary eye injury. Causes skin irritation. ... /Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

# 1.3 Average Daily Intake





Fatty acids are an important part of the normal daily diet of mammals, birds and invertebrates.

USEPA/OPPTS; R.E.D Facts. Soap Salts. Reregistration Eligibility Decisions (REDs) Database. EPA-738-F-92-013. Sept 1992. Available from the Database Query page at http://www.epa.gov/pesticides/reregistration/status.htm as of Sept 8, 2008.

Annual consumption is 1200.00 lb. Individual consumption is 0.001016 mg/kg/day.

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 1383

# 2 Emergency Medical Treatment



### 2.1 Antidote and Emergency Treatment



/SRP:/ Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Organic acids and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 176

/SRP:/ Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist respirations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Activated charcoal is not effective ... . Do not attempt to neutralize because of exothermic reaction. Cover skin burns with dry, sterile dressings after decontamination ... . /Organic acids and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 176-7

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Early intubation, at the first sign of upper airway obstruction, may be necessary. Positive-pressure ventilation techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema ... . Consider administering a beta agonist such as albuterol for severe bronchospasm ... . Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start IV administration of D5W /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors if patient is hypotensive with a normal fluid volume. Watch for signs of fluid overload ... . Use proparacaine hydrochloride to assist eye irrigation ... . /Organic acids and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 177

# 3 Animal Toxicity Studies

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### 3.1 Non-Human Toxicity Excerpts (Complete)



/LABORATORY ANIMALS: Acute Exposure/ ... Nonanoic acid (500 mg applied for 24 hr) was a moderate irritant to rabbit skin but was a severe irritant to guinea pig skin. A severe irritation was produced by applying 91 mg of the acid to rabbit eyes. No signs of toxicity were produced after inhalation of concentrated vapors by rats.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 734

/LABORATORY ANIMALS: Acute Exposure/ In a 2% emulsion based on cottonseed oil, emulsifiers and buffers, the iv LD50 of nonanoic acid in mice was found to be 244 mg/kg. The animals immediately had convulsions and collapsed on their sides and respiration ceased within 2 min, sometimes after hyperpnea.

European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) p.11 (2000 CD-ROM edition). Available from, as of January 18, 2008: http://esis.jrc.ec.europa.eu/

/LABORATORY ANIMALS: Acute Exposure/ Groups of Sprague-Dawley rats (5/sex) were exposed to aerosols containing a concentration of 0.046 or 3.8 mg/L of nonanoic acid for 4 hours. Exposure levels and particle size were measured 4 times. Animals were held for 14 day post-exposure ... LC50 between 0.46 and 3.8 mg/L (mean gravimetric exposure concn) with a nominal concentration of 0.60 and 31 mg/L, respectively. Eight (8) animals died at 3.8 mg/L. There were no mortalities at 0.46 mg/L. Signs of irritation were noted during exposure and the first week post-exposure. Survivor's recovery /was/ within 14 days ....

USEPA; High Production Volume Information System (HPVIS); Nonanoic acid ( CAS # 112-05-0). Available from, as of January 18, 2008: http://iaspub.epa.gov/oppthpv/quicksearch.display?pChem=100241

/LABORATORY ANIMALS: Acute Exposure/ The toxic, irritative, and sensitizing effects of topically applied ... nonanoic acid in methyl- or propyl ester (NAM, NAP) in the buccal mucosa were investigated in a Sprague-Dawley rat model. Semi-quantitative evaluations of cellular infiltrates were performed in routine histologic preparations. The toxic potential was tested with 2% and 0.2% solutions. All substances ... caused an increased cellularity, mainly of a mononuclear cell type. The low dose of NAM induced stronger inflammatory reactions than the high dose. Repeated applications of 2% solutions decreased the response compared to one application, except for NAM, where a clear irritative potential was observed. Pre-exposure of dorsal skin prior to buccal painting resulted in an enhanced reaction to NAM and NAP ...

#### PMID:3201116

Ahlfors EE, Larsson A; Scand J Dent Res 96(5):428-34 (1988)

/LABORATORY ANIMALS: Acute Exposure/ ... Female BALB/c mice were dermally exposed on the ears once daily for 4 consecutive days. On day 5, the lymph nodes draining the exposure sites were collected and used for RNA extraction and subsequent hybridization to Affymetrix Mu6500 oligonucleotide arrays. Of the 6519 genes on the arrays, there were 44, 13, and 51 genes in the TDI-, OXA-, and NA-exposed samples, respectively, that displayed a minimum of twofold change in expression level relative to the vehicle control. There were 32, 19, and 19 genes that were differentially expressed (with a minimum of twofold change) between TDI and OXA, TDI and NA, OXA and NA, respectively. The differentially expressed genes include immune response-related genes, transcriptional factors, signal transducing molecules, and Expressed Sequence Tags. Based on the gene array results, candidate genes were further evaluated using RT-PCR. There was only about 47% concordance between the gene array and RT-PCR results.

#### PMID:11379042

He B et al; Int Immunopharmacol 1(5):867-79 (2001)

/LABORATORY ANIMALS: Acute Exposure/ No symptoms of toxicity could be produced by inhalation of concn vapors in rats.

Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994., p. 3558

/LABORATORY ANIMALS: Acute Exposure/ Nonanoic acid is/ irritating to rabbit skin and highly irritating to rabbit

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5/11/21, 9:40 AM

eyes.

European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) p.11 (2000 CD-ROM edition). Available from, as of January 18, 2008: http://esis.jrc.ec.europa.eu/

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Nonanoic acid, fed for 4 wk @ 4.17% in diet, depressed rate of growth only in vitamin B12-deficient rats. 5% in diet was fairly well utilized by growing chicks.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 734

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ In a 28-day dermal toxicity test ... nonanoic acid (500 mg/kg) in mineral oil was applied to freshly clipped lateral and dorsal skin of New Zealand White rabbits (5/sex) daily, 5 days/week for 2 weeks. The skin of half of the animals was abraded prior to the first, sixth and eighth application. A control group was treated with mineral oil only. After 2 weeks of treatment, six animals (three with abraded and three with intact skin) were necropsied and the remaining four animals were necropsied after an additional 2-week recovery period. Tissues from 29 organs were removed for microscopic evaluation. Most animals exhibited body weight loss after one or two weeks of treatment, but animals from the recovery group showed normal weight gain. Most animals showed local dermal irritation with slight to moderate erythema, localized necrosis and exfoliation. Histopathology revealed hyperplasia, hyperkeratosis and necrosis of the skin at the application site. No other microscopic alterations were reported for any other tissue that could be related to administration of nonanoic acid. By the end of the 2-week recovery period, weight loss had disappeared and skin appeared healed ...

USEPA; SCREENING-LEVEL HAZARD CHARACTERIZATION: C7 to C9 Aliphatic Aldehydes and Carboxylic Acids Category (August 2007) p.10. Available from, as of January 16, 2008: http://www.epa.gov/hpvis/hazchar/Category\_C7-C9%20Aliphatic%20Aldehydes%20&%20Carboxylic%20Acids\_HC\_August%202007.pdf

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ Pregnant female rats (22/group) were dosed with nonanoic acid at 0 or 1500 mg/kg/day during days 6 to 15 of gestation. On Day 20 of gestation, females were sacrificed. One-third of fetuses were examined for visceral abnormalities and two-thirds were subjected to skeletal examination. There were no effects on mortality, clinical signs, body weight changes, food consumption, and gross pathology. No effects were seen on mean ovarian, uterine, litter size, pregnancy rates, corpora lutae, implantation sites, fetal viability, fetal weight, sex, gross pathology or visceral and skeletal examination. NOAEL for maternal and developmental toxicity = 1500 mg/kg/day, LOAEL > 1500 mg/kg/day.

USEPA/HPVIS; SCREENING-LEVEL HAZARD CHARACTERIZATION: C7 to C9 Aliphatic Aldehydes and Carboxylic Acids Category (August 2007) p.13. Available from, as of January 16, 2008: http://www.epa.gov/hpvis/hazchar/Category\_C7-C9%20Aliphatic%20Aldehydes%20&%20Carboxylic%20Acids\_HC\_August%202007.pdf

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ ... Each group of 25 /Xenopus/ embryos was exposed to one of 8 concentrations of /nonanoic acid/ ... Data were pooled to calculate 96 hr LC50 (lethality) and 96 hr EC50 (malformation) and development hazard index (DHI) ... LC50 = 32.7 (29 to 36) mg/L; EC50 = 6.5 (6 to 7) mg/L; DHI = 5.0 ... DHI was found to be 5 indicating a low to moderate hazard according to the authors.

USEPA; High Production Volume Information System (HPVIS); Nonanoic acid ( CAS # 112-05-0). Available from, as of January 18, 2008: http://iaspub.epa.gov/oppthpv/quicksearch.display?pChem=100241

/ALTERNATIVE and IN VITRO TESTS/ Nonanoic acid decr the contractile force of isometrically acting rat papillary muscles, with the effect depending on both concn (0.1-1 mmol) and time of exposure (2-12 min). The postextrasystolic potentiation and the time to reach a new steady state level of contraction following a paired pulse stimulation were incr by nonanoic acid.

PMID:612091

CAFFIER G, PFEIFFER C; ACTA BIOL MED GER 36 (7-8): 1077 (1977)

/GENOTOXICITY/ Five concentrations from 667 to 10,000 ug/plate of /nonanoic acid were tested in Ames assay/ ... There was no evidence that nonanoic acid was mutagenic in Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, and TA1538 with and without metabolic activation at concentrations up to 10,000 ug/plate.

USEPA; High Production Volume Information System (HPVIS); Nonanoic acid ( CAS # 112-05-0). Available from, as of January 18, 2008: http://iaspub.epa.gov/oppthpv/quicksearch.display?pChem=100241

/IMMUNOTOXICITY/ ... The /murine local lymph node assay/ proliferation induced by ... nonanoic acid ... /which is/ considered to be /a/ non-sensitiser, was further investigated ... /Nonanoic acid/ showed a dose-response relationship and clearly positive results when tested at higher concentrations (> or = 50%) and would thus be

classified as potential sensitisers according to the present criteria for a positive assay result ...

PMID:9833042

Montelius J et al; Acta Derm Venereol 78(6):433-7 (1998)

### 3.2 Ecotoxicity Excerpts (Complete)



/AQUATIC SPECIES/ PELARGONIC ACID INHIBITED CLEAVAGE OF HEMICENTROTUS PULCHERRIMUS EGGS AT A CONCN OF 200 PPM.

IWANAMI Y ET AL; CELL STRUCT FUNCT 4 (1): 67 (1979)

/OTHER TERRESTRIAL SPECIES/ Pelargonic acid inhibited pollen germination and pollen tube elongation in Camellia sinensis (tea plant).

European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) p.9 (2000 CD-ROM edition). Available from, as of January 18, 2008: http://esis.jrc.ec.europa.eu/

/PLANTS/ PELARGONIC ACID INHIBITED POLLEN GERMINATION (AVG GERMINATION 0-1.1%) AND POLLEN TUBE ELONGATION (AVG TUBE LENGTH 0-0.2 NM) IN CAMELLIA SINENSIS AND MITOTIC DIVISION OF GENERATIVE NUCLEUS IN ORNITHOGALUM VIRENS (AVG MITOSIS 0-40.6%).

IWANAMI Y, IWADARE T; BOT GAZ (CHICAGO) 140 (1): 1 (1979)

### 3.3 Non-Human Toxicity Values





LD50 Mouse oral 15000 mg/kg

European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) p.10 (2000 CD-ROM edition). Available from, as of January 18, 2008: http://esis.jrc.ec.europa.eu/

LD50 Mouse iv 224 mg/kg

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2739

LD50 Rabbit dermal >5000 mg/kg

European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) p.10 (2000 CD-ROM edition). Available from, as of January 18, 2008: http://esis.jrc.ec.europa.eu/

# 3.4 Ecotoxicity Values





LC50 Anas platyrhynchos (Mallard duck, juvenile) diet >5620 ppm for 8 days

USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on Nonanoic acid (112-05-0). Available from, as of December 27, 2007

LC50 Colinus virginianus (Northern bobwhite, juvenile) diet >5620 ppm for 8 days

USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on Nonanoic acid (112-05-0). Available from, as of December 27, 2007

LD50 Colinus virginianus (Northern bobwhite, adult) oral >2250 mg/kg for 14 days

USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on Nonanoic acid (112-05-0). Available from, as of December 27, 2007

LD50 Apis mellifera (Honey bee, worker) topical >25 ug/bee for 48 hr

USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on Nonanoic acid (112-05-0). Available from, as of December 27, 2007

EC50; Species: Xenopus laevis (African clawed frog, embryo); Conditions: freshwater, renewal, pH 7.0-7.8; Concentration: 6500 ug/L for 96 hr (6000-7000 ug/L); Effect: increased developmental changes, general (craniofacial defects, abnormal gut coiling) /> or =98% purity/

Dawson DA et al; Teratog Carcinog Mutagen 16 (2): 109-24 (1995) Available from, as of December 27, 2007

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LC50; Species: Xenopus laevis (African clawed frog, embryo); Conditions: freshwater, renewal, pH 7.0-7.8;

Concentration: 32700 ug/L for 96 hr (29000-36000 ug/L) /> or =98% purity/

Dawson DA et al; Teratog Carcinog Mutagen 16 (2): 109-24 (1995) Available from, as of December 27, 2007

EC50; Species: Daphnia magna (Water flea, age <24 hr); Conditions: freshwater, static; Concentration: 96000 ug/L for 48 hr (64000-119000 ug/L); Effect: intoxication, immobilization

USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on Nonanoic acid (112-05-0). Available from, as of December 27, 2007

LC50; Species: Lepomis macrochirus (Bluegill); Conditions: freshwater, static; Concentration: 105000 ug/L for 96 hr /99.7% purity/

USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on Nonanoic acid (112-05-0). Available from, as of December 27, 2007

LC50; Species: Oncorhynchus mykiss (Rainbow trout); Conditions: freshwater, static; Concentration: 91000 ug/L for 96 hr (68000-121000 ug/L) /99.7% purity/

USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on Nonanoic acid (112-05-0). Available from, as of December 27, 2007

LC50 Pimephales promelas (Fathead minnow, age 33 days, mean length 21.9 mm, mean weight 0.176 g) 104 mg/L for 96 hr (confidence limit: 93.4-115 mg/L); flow through, 25.3 °C, pH 7.46, dissolved oxygen 6.0 mg/L, hardness 47.0 mg/L CaCO3, alkalinity 45.0 mg/L CaCO3 /97% purity/

Brooke, L.T., D.J. Call, D.T. Geiger and C.E. Northcott (eds.). Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Superior, WI: Center for Lake Superior Environmental Studies Univ. of Wisconsin Superior, 1984., p. 349

LC50 Pimephales promelas (Fathead minnow) 104 mg/L/96 hr; static

European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) p.8 (2000 CD-ROM edition). Available from, as of January 18, 2008: http://esis.jrc.ec.europa.eu/

EC50 Pimephales promelas (Fathead minnow, age 33 days, mean length 21.9 mm, mean weight 0.176 g) 104 mg/L for 96 hr (confidence limit: 93.4-115 mg/L); flow through, 25.3 °C, pH 7.46, dissolved oxygen 6.0 mg/L, hardness 47.0 mg/L CaCO3, alkalinity 45.0 mg/L CaCO3; Effect: affected fish became hypoactive, resting on the tank bottom prior to death. /97% purity/

Brooke, L.T., D.J. Call, D.T. Geiger and C.E. Northcott (eds.). Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Superior, WI: Center for Lake Superior Environmental Studies Univ. of Wisconsin Superior, 1984., p. 349

### 3.5 TSCA Test Submissions





Nonanoic acid (CAS # 112-05-0) was evaluated for subchronic dermal toxicity and irritation in New Zealand White rabbits (5/sex/group) exposed to 500 mg/kg/day (25% w/w in mineral oil) for 5 days/week for 2 weeks. Half of the animals (3 males, 2 females) received applications upon abraded skin and half (3 females, 2 males) received applications on intact skin. Applications remained uncovered. An additional control group of 10 rabbits was treated dermally with 2 g/kg/day mineral oil. There were no mortalities throughout treatment or 2-week recovery (4 rabbits). All treated animals showed slight weight losses in the second week and food consumption was diminished in 2nd and 3rd weeks of study. Severe erythema, slight to severe edema characterized signs of irritation at the sites of application with necrosis and eschar appearing in all animals in the second week. Atonia, desquamation, fissuring and exfoliation of eschar tissue were noted as well. Treatment-related weight loss and signs of dermal irritation resolved in animals held for 2-week recovery. Upon necropsy of 6 animals (3/abraded and 3/intact) at 2 weeks, no treatment- related gross pathology was identified other than morphological changes of treated dermis. Microscopic examination revealed generally localized necrosis accompanied by epidermal hyperplasia, hyperkeratosis, and occasional diffuse and perifollicular dermal inflammation at both abraded and intact application sites. Treated rabbits held for recovery was reepithelialized and continuous with normal follicular structure and population, and with persisting mild to moderate epidermal hyperplasia and hyperkeratosis. Microscopic examination of select visceral organs from 6 rabbits at 2 weeks and 4 recovered rabbits at 4 weeks failed to expose a systemic effect of treatment.

RHONE-POULENC INC; A 28-Day Dermal Toxicity Study in Rabbits; 9/30/81; EPA Doc No. 88-920010172; Fiche No. OTS0546557

Nonanoic acid (CAS # 112-05-0) was evaluated for developmental and maternal toxicity in 22 pregnant Crl:COBS, CDBR rats administered doses of 1500 mg/kg bw by oral intubation on gestational days 6 through 15. A control group of 22 female rats received gavage doses of corn oil (vehicle). On Day 20, all rats were sacrificed for Caesarian delivery and determination of fetal/embryotoxicity and teratogenic effects, as well as fertility indices and maternal toxicity. No excess mortality, retarded bodyweight gains, decreased food consumption or other clinical signs of maternal toxicity were observed relative to control. Likewise, gross pathology upon terminal sacrifice identified no treatment-related effects in the pregnant dams. Pregnancy rates, mean number of corpora lutea, implantations, and mean implantation efficiency (implantations per corpora lutea) were comparable to controls, as were gravid and nongravid uterine weights, and mean ovarian, uterine, and litter data. Embryotoxic effects (number of resorptions, number of fetuses, fetal viability, mean fetal bodyweight, mean fetal length) were not observed. Gross pathology and skeletal examinations produced no statistically significant evidence of fetotoxicity or teratogenicity in a viable fetal population similar to that in the control group. Of 80 fetuses from 22 litters of the treated rats, there were 2 instances of cleft palate, 2 fetuses with small tongue, and a single incidence hydroureter that were not seen in control fetuses. Skeletal anomalies were likewise not statistically linked to treatment and the number of variant fetuses (2) were equal to variant controls.

RHONE-POULENC INC; Teratology Screen in Rats, Project No. 299-534; 7/28/83; EPA Doc No. 88-920009562; Fiche No. 0TS0571218

# 4 Metabolism/Pharmacokinetics



### 4.1 Metabolism/Metabolites





INFUSION OF AN EMULSION CONTAINING 20% TRINONANOATE, 0.9% SODIUM CHLORIDE, & 1% SOYBEAN LECITHINS INTO DOGS RESULTED IN OXIDN OF NONANOIC ACID.

PMID:4631028

BACH A ET AL; NUTR METAB 14 (4): 203 (1972)

NONANOIC ACID IS METABOLIZED BY THE LIVER TO PRODUCE KETONE BODIES. METABOLISM OCCURS VIA BETA-OXIDATION, AND NO EVIDENCE WAS FOUND IN RATS OF CHAIN ELONGATION OR TISSUE STORAGE OF THE ACID. METAB OF THE TERMINAL PROPIONIC ACID RESIDUE RESULTS IN INCREASED GLUCOSE AND GLYCOGEN SYNTHESIS.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 734

### 4.2 Mechanism of Action





The epidermal response to 2 different irritants, nonanoic acid (NAA) and sodium lauryl sulfate (SLS), was investigated with 2 different methods. NAA 80% and SLS 4% were applied under occlusion for up to 24 hr. Elemental changes were determined in cryosections by x-ray microanalysis. Compared to unexposed skin a significantly higher sodium/potassium ratio was found after 6 hr in NAA-exposed skin and a lower ratio in SLS-exposed. At 24 hr both substances had induced similar changes, compatible with a cell injury. The findings demonstrate a time-dependent NAA and SLS response. With reverse transcription polymerase chain reaction, the mRNA expression of interleukin-1 alpha (IL-1 alpha), -1 beta (IL-1 beta), -6 (IL-6), and -8 (IL-8), tumor necrosis factor alpha (TNF alpha) and granulocyte macrophage colony stimulating factor (GM-CSF) in shave biopsies from irritated and unexposed skin was studied at 0, 4, 8, and 24 hr. NAA, but not SLS, induced an increase in mRNA expression for IL-6. mRNA-expression for GM-CSF was increased after SLS exposure, but not after NAA. These findings indicate a time and substance dependent difference in the up-regulation of mRNA for different cytokines in epidermis during the first 24 hr of the irritants' reaction. This might be the effect of differences in the irritants action on the cell membranes, which is also reflected by the differences found in the elemental content at 6 hr.

PMID:9118630

Grängsjö A et al; Contact Dermatitis 35(6):355-60 (1996)

It has been shown that polyunsaturated fatty acids such as arachidonic and docosahexanoic acids but not monounsaturated and saturated long-chain fatty acids promote basal and nerve growth factor (NGF)-induced neurite extension of PC12 cells, a line derived from a rat pheochromocytoma. On the other hand, short-chain fatty acids and valproic acid (2-propylpentanoic acid) enhance the growth of neurite processes of the cells only in the presence of inducers. In this study, /investigators/ demonstrated that straight medium-chain fatty acids (MCFAs) at millimolar concentrations alone potently induced neuronal differentiation of PC12 cells. ... Nonanoic, decanoic, and dodecanoic acids also induced growth of neurite processes, but their maximal effects were less marked than that of octanoic acid. ...

PMID:17434686

Kamata Y et al; Neuroscience 146 (3): 1073-81 (2007)

# 5 Pharmacology





### 5.1 Therapeutic Uses



/EXPL THER/ The treatment for patients with genetic disorders of mitochondrial long-chain fatty acid beta-oxidation is directed toward providing sufficient sources of energy for normal growth and development, and at the same time preventing the adverse effects that precipitate or result from metabolic decompensation. Standard of care treatment has focused on preventing the mobilization of lipids that result from fasting and providing medium-chain triglycerides (MCT) in the diet in order to bypass the long-chain metabolic block. MCTs that are currently available as commercial preparations are in the form of even-chain fatty acids that are predominately a mixture of octanoate and decanoate. Recently, the use of odd-chain fatty acids has been proposed as an alternative treatment ... /The authors/ have shown previously that the even-numbered medium-chain fatty acids (MCFAs) that are found in MCT preparations can reduce the accumulation of potentially toxic long-chain metabolites of fatty acid oxidation (FAO). In the current study ... /they/ found that provision of odd-chain species does decrease the build-up of long-chain FAO intermediates in ... in vitro skin fibroblast model, but to a lesser extent than even-numbered MCFAs. /Odd-numbered medium-chain fatty acids (MCFAs)/

PMID:14741189

Jones PM et al; Mol Genet Metab 81(2):96-9 (2004)

### 5.2 Interactions (Complete)



Skin reactions to 40% nonanoic acid in propanol (NON) ... were evaluated by image analysis of 20 MHz B scan recordings (Dermascan C, Cortex Technology). 18 women, aged 18 to 45, were patch tested with 24-hr application time, and clinical and instrumental evaluations were performed at the beginning of the experiment, and 24 and 48 hr after patch testing. To check possible regional variations ... /NON/ was applied 2 x on the same forearm. As control tests, saline solution, propanol and sodium lauryl sulfate (SLS) 3% were applied. Echographic images were processed by a program enabling numerical representation of picture data, based on attribution of fictional values to the echoes' amplitudes, selection of amplitude bands of interest, binary transformation of the image, and calculation of the extension of areas reflecting within the same amplitude range. Sonographic recordings were evaluated by an amplitude interval marking hyporeflecting parts of the dermis (corresponding to edema and inflammatory infiltration), and by a band highlighting the entrance echo (epidermis) ... Evaluations showed that extension of the hypoechogenic area of the dermis increases according to intensity of inflammatory reaction for all irritant substances. A clear decrease in reflectivity of the epidermis echo at 24 hr was visible at SLS patch test test sites, whereas at patch test sites performed with NON ... there was a trend towards an increase in values of hyperreflecting pixels. No significant variations between data recorded at proximal compared to distal skin sites were observed ... /40% Nonanoic acid in propanol/

PMID:7821005

Seidenari S; Contact Dermatitis 31(3):146-50 (1994)

# 6 Environmental Fate & Exposure



### 6.1 Environmental Fate/Exposure Summary



Nonanoic acid's production and use in organic syntheses, lacquers, plastics, in the production of hydrotropic salts, pharmaceuticals, synthetic flavors and odors, esters for turbojet lubricants, as a flotation agent, vinyl plasticizer, and as a gasoline additive may result in its release to the environment through various waste streams. Its use as a herbicide will result in its direct release to the environment. Nonanoic acid is a fatty acid and occurs naturally in many essential oils. Fatty acids are widely distributed in nature as components of animal and vegetable fats and are an important part of the normal daily diet of mammals, birds and invertebrates. If released to air, a vapor pressure of 1.65X10-3 mm Hg at 25 °C indicates nonanoic acid will exist solely as a vapor in the atmosphere. Vapor-phase nonanoic acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 1.6 days. If released to soil, undissociated nonanoic acid is expected to have low mobility based upon an estimated Koc of 1,700 for the free acid. The pKa of nonanoic acid is 4.95, indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil surfaces is not expected to be an important fate process based upon the pKa. Biodegradation studies of nonanoic acid show a total organic carbon removal ratio of 99% using a non-acclimated activated sludge and a BOD of 0.59 (g/g) after 5 days incubation using a sewage inoculum, suggesting biodegradation is an important environmental fate in soil and water. If released into water, undissociated nonanoic acid is expected to adsorb to suspended solids and sediment based upon the estimated Koc for the free acid. The pKa indicates nonanoic acid will exist almost entirely in the anion form at pH values of 5 to 9 and therefore volatilization from water surfaces is not expected to be an important fate process. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. Occupational exposure to nonanoic acid may occur through inhalation and dermal contact with this compound at workplaces where nonanoic acid is produced or used. Monitoring data indicate that the general

# 6.2 Probable Routes of Human Exposure





NIOSH (NOES Survey 1981-1983) has statistically estimated that 76,346 workers (6,777 of these were female) were potentially exposed to nonanoic acid in the US(1). Occupational exposure to nonanoic acid may occur through inhalation and dermal contact with this compound at workplaces where nonanoic acid is produced or used (SRC). Monitoring data indicate that the general population may be exposed to nonanoic acid via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with this compound or other products containing nonanoic acid(SRC).

population may be exposed to nonanoic acid via inhalation of ambient air, ingestion of food and drinking water, and

dermal contact with this compound or other products containing nonanoic acid. (SRC)

(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available at http://www.cdc.gov/noes/ as

#### 6.3 Natural Pollution Sources





...AS AN ESTER IN OIL OF PELARGONIUM.

The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 916

...IN SEVERAL ESSENTIAL OILS, EITHER FREE OR ESTERIFIED: ROSE, GERANIUM, ORRIS, LITSEA CUBEBA, ARTEMISIA ARBORESCENS L, HOPS, CHAMAECYPARIS PISIFERA ENDL, EREMOCITRUS GLAUCA L, FRENCH LAVENDER, AND IN OAK MUSK.

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 433

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5/11/21, 9:40 AM

Nonanoic acid was identified as a volatile constituent of the kiwi fruit flower(1) and of raw earth-almond (Cyperus esculentus L.)(2). Nonanoic acid was found in fine particulate matter released (by resuspension and agitation of the leaf composites) from green and dead plant leaves at concentrations of 444.7 and 596.8 ug/g, respectively(3). The compound is a carboxylic acid that is also known as a fatty acid because fatty acids were first isolated by the hydrolysis of naturally occurring fats(4). Fatty acids are widely distributed in nature as components of animal and vegetable fats(5) including lipids such as oils and fats, waxes, sterol esters and other minor compounds(4).

(1) Tatsuka K et al; J Agric Food Chem 38: 2176-80 (1993) (2) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997) (3) Rogge WF et al; Environ Sci Technol 27: 2700-11 (1993) (4) Gutsche CD, Pasto DJ; Fundamentals of Organic Chemistry. Englewood Cliffs, NJ: Prentice-Hall p. 369 (1975) (5) Anneken DJ et al; Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (2008). NY, NY: John Wiley & Sons; Fatty Acids. Online Posting Date: Dec 15, 2006.

#### 6.4 Artificial Pollution Sources





Nonanoic acid's production and use in organic syntheses, lacquers, plastics, in the production of hydrotropic salts, pharmaceuticals, synthetic flavors and odors, esters for turbojet lubricants, as a flotation agent, vinyl plasticizer, and as a gasoline additive(1) may result in its release to the environment through various waste streams. Its use as a herbicide(2) will result in its direct release to the environment.

(1) Lewis RJ; Hawley's Condensed Chemical Dictionary. 14th Ed. NY, NY: John Wiley & Sons, Inc. p. 203 (2001) (2) USEPA; Biopesticide Active Ingredient Fact Sheets - Pelargonic Acid (217500) Fact Sheet (November 6th, 2007). Available from the Database Query page at http://www.epa.gov/oppbppd1/biopesticides/ingredients/index.htm as of January 18, 2008.

#### 6.5 Environmental Fate





TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 1,700 for the free acid(SRC), determined from a log Kow of 3.42(2) and a regression-derived equation(3), indicates that undissociated nonanoic acid is expected to have low mobility in soil (SRC). The pKa of nonanoic acid is 4.95(4), indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5). Volatilization of nonanoic acid from moist soil surfaces is not expected to be an important fate process(SRC) given the pKa. Nonanoic acid is not expected to volatilize from dry soil surfaces (SRC) based upon a vapor pressure of 1.65X10-3 mm Hg(6). Biodegradation studies of nonanoic acid show a total organic carbon removal ratio of 99% using a non-acclimated activated sludge(7), and a BOD of 0.59 (g/g) after 5 days incubation using a sewage inoculum(8), suggesting biodegradation is an important environmental fate process in soil(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Sangster J; LOGKOW Databank, Sangster Res Lab, Montreal Quebec, Canada (1994) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990) (4) Dean JA; Handbook of Organic Chemistry, NY, NY: McGraw-Hill, Inc p. 8-45 (1987) (5) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (6) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng., Washington, DC: Taylor & Francis, Vol 4 (1995) (7) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 12: 85-91 (1982) (8) Heukelekian H, Rand MC; J Water Pollut Contr Assoc 27: 1040-53 (1955)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 1,700 for the free acid(SRC), determined from a log Kow of 3.42(2) and a regression-derived equation(3), indicates that undissociated nonanoic acid is expected to adsorb to suspended solids and sediment (SRC). A pKa of 4.95(4) indicates nonanoic acid will exist almost entirely in the anion form at pH values of 5 to 9 and therefore volatilization from water surfaces is not expected to be an important fate process(5). According to a classification scheme(6), an estimated BCF of 3(SRC). from its log Kow(2) and a regression-derived equation(7), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Biodegradation studies of nonanoic acid show a total organic carbon removal ratio of 99% using a non-acclimated activated sludge(8), and a BOD of 0.59 (g/g) after 5 days incubation using a sewage inoculum(9), suggesting biodegradation is an important environmental fate process in water(SRC).

(1) Swann RL et al; Res Rev 85: 23 (1983) (2) Sangster J; LOGKOW Databank, Sangster Res Lab, Montreal Quebec, Canada (1994) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington DC: Amer Chem Soc pp. 4-9, 5-4, 5-10, 15-1 to 15-29 (1990) (4) Daubert TE, Danner RP; Physical and thermodynamic properties of pure chemicals: data compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng., Washington, DC: Taylor & Francis, Vol 4 (1995) (5) Yalkowsky SH, Dannenfelser RM; Aquasol Database of Aqueous Solubility. Version 5. College of Pharmacy, Univ of Ariz - Tucson, AZ. PC Version. (1992) (6) Dean JA; Handbook of Organic Chemistry, NY, NY, NGGraw-Hill, Inc p. 8-45 (1987) (7) Franke C et al; Chemosphere 29: 1501-14 (1994) (8) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 12: 85-91 (1982) (9) Heukelekian H, Rand MC; J Water Pollut Contr Assoc 27: 1040-53 (1955)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), nonanoic acid, which has a vapor pressure of 1.65X10-3 mm Hg at 25 °C(2), is expected to exist solely as a vapor in the ambient atmosphere. Vapor-phase nonanoic acid is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 1.6 days(SRC), calculated from its rate constant of 9.8X10-12 cu cm/molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(3). Nonanoic acid does not contain chromophores that absorb at wavelengths >290 nm and therefore is not expected to be susceptible to direct photolysis by sunlight(4).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng., Washington, DC: Taylor & Francis, Vol 4 (1995) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

#### 6.6 Environmental Biodegradation





AEROBIC: A total organic carbon reduction of 99% was observed for nonanoic acid using a non-acclimated activated sludge and an initial nonanoic acid concn of 100 mg total organic carbon/L(1). A BOD of 0.59 (g/g) was observed for nonanoic acid after 5 days incubation using a sewage inoculum(2). A 75% decrease in the initial nonanoic acid concn of 1.6 mg/L was observed after 21 days incubation in an aerobic mixed bacterial culture obtained from trench leachate at a low-level radioactive waste disposal site in West Valley, NY(3).

(1) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 12: 85-91 (1982) (2) Heukelekian H, Rand MC; J Water Pollut Contr Assoc 27: 1040-53 (1955) (3) Francis AJ; Environmental Migration of Long-lived Radionuclides, Vienna, Austria: Inter Atomic Energy Agency IAEA-SM-257/72 pp. 415-29 (1982)

ANAEROBIC: An increase of 52% in the nonanoic acid concn of 4.2 mg/L in anaerobic bacterial cultures obtained from trench leachate at a low-level radioactive waste disposal site in West Valley, NY, was attributed to the breakdown of complex compounds(1).

(1) Francis AJ; Environmental Migration of Long-lived Radionuclides, Vienna, Austria: Inter Atomic Energy Agency IAEA-SM-257/72 pp. 415-29 (1982)

# 6.7 Environmental Abiotic Degradation





The rate constant for the vapor-phase reaction of nonanoic acid with photochemically-produced hydroxyl radicals has been estimated as 9.8X10-12 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 1.6 days at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). Nonanoic acid is not expected to undergo hydrolysis in the environment due to the lack of functional groups that hydrolyze under environmental conditions(2). Nonanoic acid does not contain chromophores that absorb at wavelengths >290 nm and therefore is not expected to be susceptible to direct photolysis by sunlight(3).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 8-12 (1990)

#### 6.8 Environmental Bioconcentration





An estimated BCF of 3 was calculated in fish for nonanoic acid(SRC), using a log Kow of 3.42(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Sangster J; LOGKOW Databank, Sangster Res Lab, Montreal Quebec, Canada (1994) (2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

# 6.9 Soil Adsorption/Mobility





The Koc of undissociated nonanoic acid is estimated as 1,700 for the free acid(SRC), using a log Kow of 3.42(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that

undissociated nonanoic acid is expected to have low mobility in soil. The pKa of nonanoic acid is 4.95(4), indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

(1) Sangster J; LOGKOW Databank, Sangster Res Lab, Montreal Quebec, Canada (1994) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990) (3) Swann RL et al; Res Rev 85: 17-28 (1983) (4) Dean JA; Handbook of Organic Chemistry, NY, NY: McGraw-Hill, Inc p. 8-45 (1987) (5) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000)

#### 6.10 Volatilization from Water/Soil





A pKa of 4.95(1) indicates nonanoic acid will exist almost entirely in the anion form at pH values of 5 to 9 and therefore volatilization from water surfaces and moist soil is not expected to be an important fate process(2). Nonanoic acid is not expected to volatilize from dry soil surfaces(SRC) based upon a vapor pressure of 1.65X10-3 mm Hg(3).

(1) Dean JA; Handbook of Organic Chemistry, NY, NY: McGraw-Hill, Inc p. 8-45 (1987) (2) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (3) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation. Design Inst Phys Prop Data, Amer Inst Chem Eng., Washington, DC: Taylor & Francis, Vol 4 (1995)

#### 6.11 Environmental Water Concentrations



DRINKING WATER: Nonanoic acid was quantitatively detected in drinking water in: Cincinnati, OH in Oct 1978; New Orleans, LA in Jan 1976; Philadelphia, PA in Feb 1976; Ottumwa, IA in Sept 1976; and Seattle, WA in Nov 1976(1).

Nonanoic acid was identified in the initial survey of raw and treated water taken at waterworks treating lowland river water in the UK between March and December 1976(2). In the survey of treated water, nonanoic acid was identified in 3 of 14 samples taken between Feb and June 1979 after new treatment procedures were implemented(2).

Nonanoic acid was identified as a byproduct of chlorine dioxide disinfection of drinking water at a pilot plant in Evansville, IN(3). Nonanoic acid was identified as an ozone disinfection by-product in drinking water samples from a pilot plant in Jefferson Parish, LA which uses Mississippi River as the raw water source; samples were collected following 4 rounds of ozonation treatment performed in January, 1994, August 1994, May 1995, and September 1996(4).

(1) Lucas SV; GC/MS Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Concentrates: Vol 1 Analysis Results for 17 Drinking Water, 16 Advanced Waste Treatment and 3 Process Blank Concentrates USEPA-600/1-84-020A (NTIS PB85-128221) Columbus, OH: Columbus Labs Health Eff Res Lab (1984) (2) Fielding M et al; Organic Micropollutants in Drinking Water, TR-159, Medmenham, Eng Water Res Cent (1981) (3) Richardson SD et al; Environ Sci Technol 28: 592-99 (1994) (4) Richardson SD et al; Environ Sci Technol 33: 3368-77 (1999)

SURFACE WATER: Nonanoic acid was detected at a concn of 0.01 ppb in a water sample from the Inner Harbor Navigation Canal, Lake Pontchartain, New Orleans, LA collected at a depth of 10 m on the flood tide on June 23, 1980(1).

(1) McFall AJ et al; Chemosphere 14: 1253-65 (1985)

RAIN/SNOW: Nonanoic acid was detected in rainwater samples collected in a suburb of Hannover, Germany at an unspecified concn(1). Rain and snow samples collected from nine different locations in southern CA between 1982 and 1984 contained nonanoic acid at concns ranging from 0.007 to 0.14 uM(2). Rainwater samples collected in west Los Angeles between 1982 and 1983 contained nonanoic acid at concns ranging from 0.01 to 0.13 uM(2). Nonanoic acid was identified at 6 of 10 snow sample sites; 0.11 ug/kg at Nellim (Lapland, Finland), 0.12 ug/kg at Muonio (Lapland, Finland), 0.56 ug/kg at Levi (Lapland, Finland), 0.05 ug/kg at Butovo (Moscow, Russia), 0.53 ug/kg at Moscow State University (Moscow, Russia), and 1.51 ug/kg at Baikal'sk (Lake Baikal, Siberia)(3).

(1) Winkeler HD et al; Vom Wasser 70: 107-17 (1988) (2) Kawamura K et al; Atmos Environ 30: 1035-52 (1996) (3) Poliakova OV et al; Toxicol Environ Chem 75: 181-94 (2000)

#### 6.12 Effluent Concentrations





Nonanoic acid was detected in aqueous industrial effluent extracts collected between Nov 1979-81 in the following industrial categories (concentration in one effluent extract): ore mining (12 ng/uL); auto and other laundries (34

ng/uL); porcelain/enameling (28 ng/uL); electronics (3084 ng/uL); mechanical products (1954 ng/uL); and publicly owned treatment works at an unknown concn(1). Nonanoic acid was identified in the acidic fraction of sewage and sludge from the Iona Island Sewage Treatment Plant, British Columbia(2). The acidic fraction of oil shale retort water from the Kerosene Creek seam of the Rundle deposit, Queensland, Australia, was found to contain nonanoic acid at a concn of 200 mg/L(3). A grab sample, obtained in April 1980, of the final effluent from the Addison, IL Publicly Owned Treatment Works was found to contain nonanoic acid at an unreported concn(4). Groundwater samples contaminated by industrial pollution near Barcelona, Spain were found to contain nonanoic acid at concns ranging from <5 to 75 ng/L(5). Nonanoic acid was detected in trench leachate from a low-level radioactive waste disposal site in West Valley, NY at an average concn of 4.5 mg/L(6). Nonanoic acid was detected in process retort water from the Occidental Oil Shale, Inc facility in Logan Wash, CO at a concn of 81 mg/L(7). Nonanoic acid was detected in: process water from in situ coal gasification in Gillette, WY at a concn of 5 ppm; retort water from in situ oil shale processing in Rock Springs, WY at a concn of 493 ppm; and boiler blowdown water from in situ shale oil processing in DeBeque, CO at a concn of 132 ppm(8). Nonanoic acid was detected in emissions from a municipal waste incineration plant at an unspecified concn(9).

(1) Bursey JT, Pellizzari ED; Analysis of Industrial Wastewater for Organic Pollutants in Consent Degree Survey, Contract No. 68-03-2867, Athens, GA: USEPA Environ Res Lab (1982) (2) Rogers IH et al; Water Pollut Res J Canada 21: 187-204 (1986) (3) Dobson KR et al; Water Res J 19: 849-56 (1985) (4) Ellis DD et al; Arch Environ Contam Toxicol 11: 373-82 (1982) (5) Guardiola J et al; Water Supply 7: 11-16 (1989) (6) Francis AJ et al; Nuclear Tech 50: 158-63 (1980) (7) Leenheer JA et al; Environ Sci Technol 16: 714-23 (1982) (8) Pellizzari ED et al; Identification of organic components in aqueous effluents from energy-related processes. ASTM Spec Tech Publ. STP 686 pp. 256-73 (1979) (9) Jay K, Stieglitz L; Chemosphere 30: 1249-60 (1995)

Nonanoic acid was emitted from medium duty diesel trucks at 240 ug/km(1). Nonanoic acid was measured in the emissions of gasoline powered motor vehicles at a rate of 27.9 ug/km and 80.6 ug/km for catalyst equipped engines and non-catalyst equipped engines(2). Fine aerosol emission rates of nonanoic acid from heavy-duty diesel trucks, noncatalyst-equipped, and catalyst-equipped automobiles were 146.9, 8.6, and 196.2 ug/km, respectively(3).

Nonanoic acid was detected in road dust particles collected from paved streets in a residential area of Pasadena, CA in May 1988 at a concn of 135.4 ug/g of particle sample; brake lining particles at a concn of 87.4 ug/g of particle sample; and tire wear particles at a concn of 90.9 ug/g of particle sample(4). Nonanoic acid was detected in exhaust from a gasoline engine at a concn of 0.052 ppb(5).

(1) Schauer JJ et al; Environ Sci Technol 33:1578-87 (1999) (2) Schauer JJ et al; Environ Sci Technol 36: 1169-80 (2002) (3) Rogge WF et al; Environ Sci Technol 27: 636-51 (1993) (4) Rogge WF et al; Environ Sci Technol 27: 1892-904 (1993) (5) Kawamura K et al; Environ Sci Technol 19: 1082-6 (1985)

Nonanoic acid was identified as a fine particle released from a natural gas-fired space heater and water heater; emission rates were 225.2 pg/kJ and 482.6 pg/kJ for the first series of filters and backup filters within the samplers, respectively(1). Nonanoic acid was found in candle smoke from paraffin and beeswax at 0.25 and 0.31 mg/g of organic compounds(2). Nonanoic acid was found in the fine aerosols from boilers burning number 2 distillate fuel oil at a rate of 184.8 pg/kJ (burning at 58% capacity with 6.5% excess oxygen in stack gases) and not detected (burning at 54% capacity with 7.1% excess oxygen in stack gases)(3). Nonanoic acid was not detected in wood smoke from pine, and detected in smoke from oak and synthetic logs at 0.24 and 0.97 mg/kg of wood burnt(4). Nonanoic acid was found at 1312 ug/g from heated roofing tar pot fumes(5). Nonanoic acid was found in gas and particulate matter effluents from commercial-scale meat charbroiling operations at 42,400 and 6,030 ug/kg meat cooked, respectively(6).

(1) Rogge WF et al; Environ Sci Technol 27: 2736-44 (1993) (2) Fine PM et al; Environ Sci Technol 33: 2352-62 (1999) (3) Rogge WF et al; Environ Sci Technol 31: 2731-7 (1997) (4) Rogge WF et al; Environ Sci Technol 32: 13-22 (1998) (5) Rogge WF et al; Environ Sci Technol 31: 2726-30 (1997) (6) Schauer JJ et al; Environ Sci Technol 33: 1566-77 (1999)

# 6.13 Sediment/Soil Concentrations



SEDIMENT: Nonanoic acid was detected, not quantified in sediment samples collected from Dokai Bay, Japan on Sept 28 1990(1). Nonanoic acid was identified in sediment samples taken Sept 1995 at the mouth of 3 rivers and in 1 port in Niigata, Japan(2).

(1) Terashi A et al; Bull Environ Contam Toxicol 50: 348-55 (1993) (2) Kawata K et al; Bull Environ Contam Toxicol 65: 660-7 (2000)

#### 6.14 Atmospheric Concentrations





URBAN/SUBURBAN: Nonanoic acid was identified in air samples collected along the Niagara River in Sept 1982 at an unreported concn(1). The average ambient annual concn of nonanoic acid in fine particles collected from West Los Angeles, downtown Los Angeles, Pasadena, and Rubidoux,, CA in 1982 was 3.3, 6.6, 5.3, and 9.9 ng/cu m, respectively(2). Nonanoic acid had an average concentration of 4.9 ng/cu m in 4 urban sites from southern CA from samples taken Sept 8-9, 1993(3). Nonanoic acid was found at 0.002-0.009, 0.002-0.008, 0.007-0.013, and 0.005-0.006 ppbv at UCLA campus, Newberry Park, Monterey Park, and La Habra, CA in Oct 1984(4). Air samples collected in Los Angeles between July and Sept 1984 contained 0.0009 to 0.011 ppb nonanoic acid(5). Nonanoic acid was detected at 0.09, 0.11, 0.14 and 0.13 ug/cu m in Long Beach, Los Angeles, Azusa and Claremont, CA, respectively, Sept 8-9, 1993(6).

(1) Hoff RM, Chan K; Environ Sci Technol 21: 556-61 (1987) (2) Rogge WF et al; Atmos Environ 27A: 1309-30 (1993) (3) Fraser MP et al; Environ Sci Technol 37: 446-53 (2003) (4) Kawamura K et al; Atmos Environ 34: 4175-91 (2000) (5) Kawamura K et al; Environ Sci Technol 19: 1082-6 (1985) (6) Nolte CG et al; Environ Sci Technol 33: 540-5 (1999)

RURAL/REMOTE: The average ambient annual concn of nonanoic acid in fine particles collected from San Nicolas Island, CA in 1982 was 0.24 ng/cu m(1). Nonanoic acid was detected at 0.01 ug/cu m on San Nicolas Island, CA, Sept 8-9, 1993(2). Nonanoic acid was detected at an unreported concn in air samples collected in a spruce forest in Eggegebirge, North-Rhine Westphalia(3). Remote aerosol samples collected from the North Pacific Ocean, heavily vegetated areas of American Samoa, and the Marshall Islands contained a nonanoic acid concn of 0.031, 4.91, and 0.060 mg/cu m, respectively(4).

(1) Rogge WF et al; Atmos Environ 27A: 1309-30 (1993) (2) Nolte CG et al; Environ Sci Technol 33: 540-5 (1999) (3) Helmig D et al; Chemosphere 19: 1399-1412 (1989) (4) Kawamura K, Gagosian RB; Nature 325: 330-1 (1987)

#### 6.15 Food Survey Values





Nonanoic acid was identified as a volatile component of raw beef(1). Nonanoic acid has been identified as a volatile flavor component of mutton and beef(2). Aerosol emission rates of nonanoic acid from frying hamburger meat was 10.2 mg/kg of meat cooked; emission rates from charbroiling hamburger was 30.6 mg/kg of meat cooked for extra lean hamburger (approx. 10.0% fat) and 47.1 mg/kg of meat cooked for regular hamburger (approx. 21% fat)(3). Nonanoic acid was found in popcorn using wet extraction method at 29 ug/kg(4). Nonanoic acid was detected, not quantified as a volatile component of raw and roasted earth-almond (Cyperus esculentus L.)(5). Nonanoic acid was found in gas and particulate matter effluents from commercial-scale meat charbroiling operations at 42,400 and 6,030 ug/kg meat cooked, respectively(6).

(1) King MF et al; J Agric Food Chem 41: 1974-81 (1993) (2) Shahidi F et al; CRC Crit Rev Food Sci Nature 24: 141-243 (1986) (3) Rogge WF et al; Environ Sci Technol 25: 1112-25 (1991) (4) Buttery RG et al; J Agric Food Chem 45: 837-43 (1997) (5) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997) (6) Schauer JJ et al; Environ Sci Technol 33: 1566-77 (1999)

#### 6.16 Plant Concentrations





Nonanoic acid was identified as a volatile constituent of the kiwi fruit flower(1). Nonanoic acid was found in fine particulate matter released (by resuspension and agitation of the leaf composites) from green and dead plant leaves at concns of 444.7 and 596.8 ug/g, respectively(2). Nonanoic acid was found as a volatile component of raw earthalmond (Cyperus esculentus L.)(3).

(1) Tatsuka K et al; J Agric Food Chem 38: 2176-80 (1993) (2) Rogge WF et al; Environ Sci Technol 27: 2700-11 (1993) (3) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997)

# 6.17 Fish/Seafood Concentrations





Nonanoic acid was detected in fresh mussels obtained from the Oarai Coast in Ibaraki, Japan at a concn of 0.08 ug/g wet weight(1).

(1) Yashuara A; J Chromatogr; 409: 251-8 (1987)

#### 6.18 Other Environmental Concentrations





Dust samples collected from 12 households in three urban areas of central Finland contained nonanoic acid at an unreported concn(1). Nonanoic acid was found in unburned paraffin and beeswax at 0.33 and 0.30 mg/g of wax(2).

(1) Hirvonen A et al; Indoor Air 4: 255-64 (1994) (2) Fine PM et al; Environ Sci Technol 33: 2352-62 (1999)

# 7 Environmental Standards & Regulations



#### 7.1 FDA Requirements



Nonanoic acid is a food additive permitted for direct addition to food for human consumption as a synthetic flavoring substance and adjuvant in accordance with the following conditions: a) they are used in the minimum quantity required to produce their intended effect, and otherwise in accordance with all the principles of good manufacturing practice, and 2) they consist of one or more of the following, used alone or in combination with flavoring substances and adjuvants generally recognized as safe in food, prior-sanctioned for such use, or regulated by an appropriate section in this part.

21 CFR 172.515 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 1, 2008: http://www.ecfr.gov

# 8.1 Molecular Formula C9-H18-O2 8.2 Molecular Weight 158.24 Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-398 8.3 Color/Form Colorless, oily liquid at ordinary temp; crystallizes when cooled

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1220

#### Yellowish oil

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 841

# 

#### **FATTY ODOR**

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 433

#### COCONUT AROMA

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Volume 2. Boca Raton, Florida: CRC Press, Inc., 1980., p. 293

#### Slight odor

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 841

# 8.5 Taste

#### UNPLEASANT TASTE

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 433

#### **EXCELLENT COCONUT TASTE**

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Volume 2. Boca Raton, Florida: CRC Press, Inc., 1980., p. 293

# 8.6 Boiling Point ② 🖸

#### 254.5 °C

Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-398

# 8.7 Melting Point ② 🖸

12.4 °C

Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-398

# 8.8 Density



0.9052 g/cu cm at 20 °C

Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-398

#### 8.9 Heat of Combustion



-5,456.1 kJ/mol

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V5:

### 8.10 LogP



log Kow = 3.42

Sangster J; LOGKOW Databank, Sangster Res Lab, Montreal Quebec, Canada (1994)

# 8.11 Solubility





Soluble in ethanol, chloroform, ether

Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-398

1:8 IN 50% ALCOHOL; 1:3 IN 60% ALCOHOL; INSOL IN WATER; SOL IN MOST ORG SOLVENTS

Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 433

In water, 284 mg/L at 30 °C

Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 375

# 8.12 Vapor Density





4.41 (Air = 1)

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 10th ed. Volumes 1-3 New York, NY: John Wiley & Sons Inc., 1999., p. V3: 2739

# 8.13 Vapor Pressure





1.65X10-3 mm Hg at 25 °C

Daubert, T.E., R.P. Danner. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis, 1989.

# 8.14 Viscosity





8.08 mPa.sec at 20 °C

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V5: 149 (1993)

#### 8.15 Refractive Index





Index of refraction: 1.4343 at 20 °C/D

Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-398

### 8.16 Other Experimental Properties





Boiling point = 255.6 °C

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 841

Acid value: 351 mg KOH/g

Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 665

Specific heat: 2.91 J/g (for the solid); Heat of fusion: 20.3 kJ/mol.

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V5: 149 (1993)

Henry's Law constant = 1.62X10-6 atm-cu m/mole at 25 °C (est)

SRC; The Physical Properties Database (PHYSPROP). Syracuse, NY: Syracuse Res Corp. Available from, as of Dec 18, 2007: http://www.syrres.com/esc/physprop.htm

Hydroxyl radical reaction rate constant = 9.76X10-12 cu cm/molec-sec at 25 °C (est)

US EPA; Estimation Program Interface (EPI) Suite. Ver.3.12. Nov 30, 2004. Available from, as of Dec 18, 2007: http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

9 Spectral Information 9.1 1D NMR Spectra		<b>?</b> Z
		<b>?</b> Z
1D NMR Spectra	1H NMR: 9 (Sadtler Research Laboratories Spectral Collection)	
9.1.1 13C NMR Spectra		<b>?</b> Z
13C NMR Spectra	13C NMR: 362 (Johnson & Jankowski, Carbon-13 NMR Spectra, John Wiley & Sons, N	NY)
9.2 Mass Spectrometry		<b>?</b> Z
9.2.1 Other MS		<b>?</b> Z
Other MS	MASS: 5504 (NIST/EPA/MSDC Mass Spectral database, 1990 version)	
9.3 IR Spectra		<b>?</b> Z
IR Spectra	IR: 60 (Sadtler Research Laboratories Prism Collection)	

# 10 Chemical Safety & Handling

#### 10.1 Odor Threshold

Aroma threshold values: Detection: 3 to 9 ppm.

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 1383

#### 10.2 Fire Potential



Combustible

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 951

#### 10.3 Flash Point



133 °C (open cup)

European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) p.6 (2000 CD-ROM edition). Available from, as of January 18, 2008: http://esis.jrc.ec.europa.eu/

#### 10.4 Explosive Limits and Potential



Combustible

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 951

#### 10.5 Preventive Measures





SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

SRP: Contaminated protective clothing should be segregated in such a manner so that there is no direct personal contact by personnel who handle, dispose, or clean the clothing. Quality assurance to ascertain the completeness of the cleaning procedures should be implemented before the decontaminated protective clothing is returned for reuse by the workers. Contaminated clothing should not be taken home at end of shift, but should remain at employee's place of work for cleaning.

Agricultural Use Requirements: Use this product only in accordance with its labeling and with the Worker Protection Standard.... Do not enter or allow worker entry into treated areas during the restricted entry interval (REI) of 12 hours. ./Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

Do not get in eyes, on skin or on clothing. Avoid breathing spray mist. Wash thoroughly with soap and water after handling. Pemove contaminated clothing and wash clothing before reuse. /Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

Worker Protection Standard Uses: Discard clothing and other absorbent materials that have been drenched or heavily contaminated with this product's concentrate. Do not reuse them. Follow manufacturer's instructions for cleaning/maintaining personal protective equipment (PPE). If no such instructions for washables, use detergent and hot water. Keep and wash PPE separate from other laundry../Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

Users should wash hands before eating, drinking, chewing gum, using tobacco or using the toilet. Remove clothing immediately if pesticide gets inside. Then wash thoroughly and put on clean clothing. Remove personal protective equipment (PPE) immediately after handling this product. Wash the outside of gloves before removing. As soon as possible, wash thoroughly and change into clean clothing. /Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

If in eyes: hold eye open and rinse slowly and gently with water for 15-20 minutes. Remove contact lenses, if present, after the first 5 minutes, then continue rinsing eye. ... If on skin or clothing: Take off contaminated clothing. Rinse skin immediately with plenty of water for 15-20 minutes. ... /Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

Care must be exercised to avoid contact of spray with foilage of desirable turfgrasses, trees, shrubs, or other desirable vegetation since damage can result. /Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

# 10.6 Storage Conditions





Do not contaminate water, food, or feed by storage... . Keep conatiner tightly sealed when not in use. Store only in original container in a dry place inaccessible to children and pets. /Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

#### 10.7 Disposal Methods





SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

Do not contaminate water, food, or feed by ... disposal. ... Pesticide disposal:: Wastes resulting from the use of this product must be disposed of on site or at an approved waste disposal facility. Container disposal: Do not reuse empty container. Triple rinse, then offer for recycling or reconditioning, or puncture and dispose of in a sanitary landfill or by incineration, or if allowed by state and local authorities, by burning. If burned, stay out of smoke. /Scythe herbicide (57% pelargonic acid)/

Dow AgroSciences; Scythe Herbicide Specimen Label. Label Code: Do2-305-002. 5 p. (February 3, 2006 revision)

# 11 Manufacturing/Use Information



#### 11.1 Uses



For Nonanoic acid (USEPA/OPP Pesticide Code: 217500) ACTIVE products with label matches. /SRP: Registered for use in the U.S. but approved pesticide uses may change periodically and so federal, state and local authorities must be consulted for currently approved uses./

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

Organic synthesis, lacquers, plastics, production of hydrotropic salts, pharmaceuticals, synthetic flavors and odors, flotation agent, esters for turbojet lubricants, vinyl plasticizer, gasoline additive.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 951

#### CHEM INT FOR NONANOYL CHLORIDE

SRI

CHEM INT FOR SPECIALTY DIESTERS-EG, WITH PROPYLENE GLYCOL

SRI

Pelargonic acid ... is used as an herbicide to prevent growth of weeds both indoors and outdoors, and as a blossom thinner for apple and pear trees ... can also be used as a sanitizer.

USEPA; Biopesticide Active Ingredient Fact Sheets - Pelargonic Acid (217500) Fact Sheet (November 6th, 2007). Available from, as of January 18, 2008: http://www.epa.gov/oppbppd1/biopesticides/ingredients/index.htm

The Food and Drug Administration (FDA) has approved pelargonic acid as a food additive, and as an ingredient in solutions used commercially to peel fruits and vegetables.

USEPA; Biopesticide Active Ingredient Fact Sheets - Pelargonic Acid (217500) Fact Sheet (November 6th, 2007). Available from, as of January 18, 2008: http://www.epa.gov/oppbppd1/biopesticides/ingredients/index.htm

#### Reported uses (ppm):

Table: Reported uses (ppm): (Flavor and Extract Manufacturers' Association)

Food Category	Usual	Max.
Alcoholic beverages	1.00	3.00
Baked goods	10.04	23.54
Fats, oils	1.00	10.00
Frozen dairy	2.14	9.38
Gelatins, puddings	1.91	5.73
Meat products	6.50	13.10
Nonalcoholic beverages	1.03	2.38
Soft candy	1.57	4.99

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 1383

#### 11.2 Manufacturers



Cognis Oleochemicals LLC, 4900 Este Ave., Cincinnati, OH 45232, (513) 482-2100; Production site: Cincinnati, OH 45232

SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 603

Oxea Corp., 1603 West LBJ Freeway, P.O. Box 810349, Dallas, TX 75381, (972) 443-8900; Production site: Bay City,

#### TX 77404

SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 603

Penta Manufacturing Co., 50 Okner Pkwy., Livingston, NJ 07039-1604, (973) 740-2300; Production site: East Hanover, NJ 07936

SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 603

Dow Agrosciences LLC, 9330 Zionsville Rd, 308/2E, Indianapolis IN 46268 Pesticide registrant/

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

Monsanto, 13th St.NW, Suite 660, Washington DC 20005 /Pesticide registrant/

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

West Agro Inc, 11100 N. Congress Ave, Kansas City MO 64153 / Pesticide registrant/

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

Ecolab Inc., 379 Wabasha St., Ecolab Center, St. Paul MN 55102 / Pesticide registrant/

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

# 11.3 Methods of Manufacturing





Prepn from unsaturated hydrocarbons by the oxo process: Hill, U.S. pat 2,815,355 (1957 to Standard Oil of Indiana); from tall oil unsaturated fatty acids: Maggiolo, U.S. pat 2,865,937 (1958 to Welsbach); by oxidation of oleic acid: Mackenzie, Morgan, U.S. pat 2,820,046 (1958 to Celanese); from rice bran oil fatty acid: Mihara et al, U.S. pat 3,060211 (1962 to Toya Koatsu Ind). Purification: Port, Reiser, U.S. pat 2,890,230 (1959 to U.S.D.A.).

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 1220

By oxidation of methylnonyl ketone; by oxidation of oleic acid; or from heptyl iodide via malonic ester synthesis.

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 1383

By oxidation of nonyl alcohol or nonyl aldehyde; the oxidation of oleic acid, especially by ozone.

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 951

# 11.4 General Manufacturing Information





FLAVORS USEFUL IN COCONUT, BERRY.

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Volume 2. Boca Raton, Florida: CRC Press, Inc., 1980., p. 293

PELARGONIC ACID SHOWED STRONG ANTIBACTERIAL ACTIVITY AGAINST STREPTOCOCCUS FAECALIS IN SILKWORM LARVAE.

IIZUKA T ET AL; J FAC AGRIC, HOKKAIDO UNIV 59 (2): 262 (1979)

PLAQUE SAMPLES COLLECTED AFTER A NONANOATE-GLUCOSE MOUTH RINSE @ PH 8.0 SHOWED LESS ACID FORMATION AND GLYCOLYSIS. NONANOATE IS EFFECTIVE IN THE PRESENCE OF SUGAR IN INHIBITING GLYCOLYSIS & PREVENTING LOW PH PRODN FROM CARBOHYDRATES WHICH ARE LIKELY TO BE HIGHLY CARIOGENIC.

PMID:6947730

HAYES ML; ARCH ORAL BIOL 26 (3): 223 (1981)

#### FEMA NUMBER 2784

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 904

COMPOSITIONS CONTAINING PELARGONIC ACID ARE ATTRACTANTS FOR TABAKOSHIBANMUSHI (A PEST INSECT THAT INFESTS STORED FOODS AND TOBACCO).

TABAKOSHIBANMUSHI ATTRACTANTS; JPN KOKAI TOKKYO KOHO PATENT NO 82 72901 05/07/82 (JAPAN TOBACCO AND SALT PUBLIC CORP)

... In 1980, it was suggested that nonanoic acid (NNA) could be used as a positive control when patch testing. Since then, NNA has been used as an experimental irritant in several studies and has been used as a chemically different substance compared to Sodium lauryl sulfate (SLS) ...

PMID:14678207

Wahlberg JE, Lindberg M; Contact Dermatitis 49(3):117-23 (2003)

# 11.5 Formulations/Preparations (Complete)



Grade: Technical 99%

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 951

Econosan Acid Sanitizer: Active Ingredients 8.50% Phosphoric acid, 10.0% Propionic acid, 9.50% Sulfuric acid, 3.00% Capric acid; 3.00% Nonanoic acid

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

Mandate Plus: Active Ingredients 1.09% Capric acid and 6.30% Nonanoic acid

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

MON 78999 Herbicide: Active Ingredients 2.00% Glyphosate, isopropylamine salt, and 2.00% Nonanoic acid

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

RD 1653 Herbicide: Active Ingredients 1.00% Glyphosate, isopropylamine salt; 0.017% Imazaquin, monoammonium salt; 2.00% Nonanoic acid

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

RD 1662 Herbicide: Active Ingredients 1.00% Glyphosate, isopropylamine salt; 0.100% Triethylamine triclopyr; 2.00% Nonanoic acid

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

Scythe Herbicide: Active Ingredient 57.0% Nonanoic acid

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

West Agro Acid Sanitizer: Active Ingredients 28.5% Phosphoric acid, 10.0% Propionic acid, 3.00% Capric acid, 3.00% Nonanoic acid

National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Nonanoic acid (112-05-0). Available from, as of February 6, 2008: http://npirspublic.ceris.purdue.edu/ppis/

EC.

Tomlin CDS, ed. Nonanoic acid (112-05-0). In: The e-Pesticide Manual, 13th Edition Version 3.2 (2005-06). Surrey UK, British Crop Protection Council.

Biopesticide (Non-systemic, broad-spectrum contact herbicide): Ammonium nonanoate (PC code 031802; the end use product contains 40.0% by weight ammonium nonanoate; Trade name: Racer Concentrate; Formulation Type: Liquid)

USEPA/Office of Pesticide Programs; Biopesticide Registration Action Document - Ammonium nonanoate p.6 AMS-TM-07-0032-0042.1 (March 16, 2007). Available from, as of March 11, 2008: http://www.regulations.gov/search/Regs/home.html#home

#### 11.6 U.S. Production



(1980) 9.75X10+9 GRAMS (EST CONSUMPTION)

SRI

(1981) PROBABLY GREATER THAN 6.81X10+6 GRAMS

SR

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year Production Range (pounds)

Year	Production Range (pounds)
1986	>10 million - 50 million
1990	>10 million - 50 million
1994	>10 million - 50 million
1998	>10 million - 50 million
2002	>10 million - 50 million

US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). Nonanoic Acid (112-05-0). Available from, as of January 14, 2008: http://www.epa.gov/oppt/iur/tools/data/2002-vol.html

Nonanoic acid is listed as a High Production Volume (HPV) chemical (65FR81686). Chemicals listed as HPV were produced in or imported into the U.S. in >1 million pounds in 1990 and/or 1994. The HPV list is based on the 1990 Inventory Update Rule. (IUR) (40 CFR part 710 subpart B; 51FR21438).

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program. Available from the Database Query page at: http://www.epa.gov/hpv/pubs/general/opptsrch.htm on Nonanoic Acid (112-05-0) as of February 4, 2008

# 12 Laboratory Methods



#### 12.1 Clinical Laboratory Methods



Analyte: nonanoic acid; matrix: blood (plasma); procedure: high-performance liquid chromatography with fluorescence detection at 365 nm (excitation) and 460 nm (emission); limit of quantitation: 5 pmole

Tsuchiya H et al; J Chromatogr 309: 43-52 (1984). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)

Analyte: nonanoic acid; matrix: blood (serum); procedure: high-performance liquid chromatography with fluorescence detection at 350 nm (excitation) and 530 nm (emission)

Yanagisawa I et al; J Chromatogr 345: 229-240 (1985). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)

# 12.2 Analytic Laboratory Methods (Complete)



SIMULTANEOUS GAS CHROMATOGRAPHIC SEPARATION OF A MIXT OF FATTY ACIDS, PHENOLS AND INDOLES INCL NONANOIC ACID IN CIGARETTE SMOKE IS DESCRIBED.

PMID:925108

HOSHIKA Y; J CHROMATOGR 144 (2): 181 (1977)

# 13 Special References



# 13.1 Special Reports



European Chemicals Bureau; IUCLID Dataset, Nonanoic acid (CAS # 112-05-0) (2000 CD-ROM edition). Available from the Database Query page at: http://ecb.jrc.it/esis/esis.php as of January 18, 2008.

USEPA/HPVIS; SCREENING-LEVEL HAZARD CHARACTERIZATION: C7 to C9 Aliphatic Aldehydes and Carboxylic Acids Category (August 2007) Available from http://www.epa.gov/hpvis/hazchar/Category\_C7-C9%20Aliphatic%20Aldehydes%20&%20Carboxylic%20Acids\_HC\_August%202007.pdf as of January 16, 2008.

# 14 Synonyms and Identifiers **Synonyms** 112-05-0 NONANOIC ACID CIRRASOL 185A **EMFAC 1202** Hexacid C-9 N-NONANOIC ACID NONOIC ACID N-NONOIC ACID NONYLIC ACID N-NONYLIC ACID 1-Octane carboxlic acid 1-Octanecarboxylic acid OCTANE-1-CARBOXYLIC ACID PELARGIC ACID N-Pelargonic acid PELARGONIC ACID PELARGON (RUSSIAN) USEPA/OPP Pesticide Code: 217500 14.1 Related HSDB Records 14.2 Substance Title

NONANOIC ACID

# 15. Administrative Information 15.1 Hazardous Substances DataBank Number 5554 15.2 Last Revision Date 20081007 15.3 Last Review Date Reviewed by SRP 5/8/2008

15.4 Update History Complete Update on 2008-10-07, 63 fields added/edited/deleted Complete Update on 02/14/2003, 1 field added/edited/deleted. Complete Update on 11/08/2002, 1 field added/edited/deleted. Complete Update on 08/06/2002, 1 field added/edited/deleted. Complete Update on 01/14/2002, 1 field added/edited/deleted. Complete Update on 08/09/2001, 1 field added/edited/deleted. Complete Update on 05/15/2001, 1 field added/edited/deleted. Complete Update on 06/12/2000, 1 field added/edited/deleted. Complete Update on 02/08/2000, 1 field added/edited/deleted. Complete Update on 02/02/2000, 1 field added/edited/deleted. Complete Update on 09/21/1999, 1 field added/edited/deleted. Complete Update on 08/27/1999, 1 field added/edited/deleted. Complete Update on 06/03/1998, 1 field added/edited/deleted. Complete Update on 03/10/1998, 1 field added/edited/deleted. Complete Update on 12/15/1997, 32 fields added/edited/deleted. Field Update on 11/01/1997, 1 field added/edited/deleted. Complete Update on 04/23/1997, 6 fields added/edited/deleted. Complete Update on 03/17/1997, 34 fields added/edited/deleted. Complete Update on 01/30/1996, 1 field added/edited/deleted. Complete Update on 01/05/1995, 1 field added/edited/deleted. Complete Update on 04/04/1994, 1 field added/edited/deleted. Field update on 01/08/1993, 1 field added/edited/deleted. Complete Update on 10/10/1990, 1 field added/edited/deleted. Complete Update on 04/16/1990, 1 field added/edited/deleted.

Field update on 12/29/1989, 1 field added/edited/deleted.

Complete Update on 01/16/1985

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