

US EPA ARCHIVE DOCUMENT



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

February 22, 2005

ACTION MEMORANDUM

SUBJECT: Inert Ingredient Tolerance Reassessment - Gluconic Acid and Sodium Salt

FROM: Dan Rosenblatt, Chief
Minor Use, Inerts, and Emergency Response Branch

TO: Lois A. Rossi, Director
Registration Division

I. FQPA REASSESSMENT ACTION

Action: Reassessment of one (1) inert ingredient exemption from the requirement of a tolerance.

Chemical and Use Summary: See table below.

Tolerance Exemption Being Reassessed				
Tolerance Exemption Expression	CAS Reg No.	40 CFR §	Use Pattern (Pesticidal)	List Classification
Gluconic acid and sodium salt	133-42-6 (gluconic acid)	180.920 ^{1/}	Sequestrant	3
	526-95-4 (D-gluconic acid)			3
	527-07-1 (sodium gluconate)			4B
	14906-97-9 (D-gluconic acid, sodium salt)			not listed

1. Residues listed in 40 CFR §180.920 [formerly 40 CFR§ 180.100(d)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to growing crops only.

List Reclassification Determination: Gluconic acid and D-gluconic acid are classified as List 3 inert ingredients, sodium gluconate is classified as a List 4B inert ingredient, and D-gluconic acid, sodium salt has not been categorized as to inert ingredient list classification status. Based upon the determination that these substances are of very low toxicity, gluconic acid, D-gluconic acid, sodium gluconate and D-gluconic acid, sodium salt can be reclassified as List 4A inert ingredients.

II. MANAGEMENT CONCURRENCE

I concur with the reassessment of the one (1) exemption from the requirement of a tolerance for the inert ingredient gluconic acid and sodium salt, and with the list reclassification determination for gluconic acid, D-gluconic acid, sodium gluconate and D-gluconic acid, sodium salts, as described above. I consider the one (1) exemption from the requirement of a tolerance for established in 40 CFR §180.920 [formerly 40 CFR§180.1001(d)] for gluconic acid and sodium salt to be reassessed as of the date of my signature, below. A Federal Register Notice regarding this tolerance exemption reassessment decision will be published in the near future.



Lois A. Rossi, Director
Registration Division

Date: _____

2/25/05

cc: Debbie Edwards, SRRD
Joe Nevola, SRRD



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MEMORANDUM

SUBJECT: Reassessment of the Exemption from the Requirement of a Tolerance for
Gluconic Acid and Sodium Salt

FROM: Kerry Leifer, Inerts Team Leader
Minor Use, Inerts and Emergency Response Branch
Registration Division (7505C)

TO: Dan Rosenblatt, Chief
Minor Use, Inerts and Emergency Response Branch
Registration Division (7505C)

Background

Attached is the science assessment for gluconic acid and sodium salt. This assessment summarizes available information on the use, physical/chemical properties, toxicological effects, exposure profile, and environmental fate and ecotoxicity of gluconic acid and sodium gluconate. In performing this assessment, EPA has relied extensively upon peer-reviewed evaluations performed by the Joint Expert Committee on Food Additives of the Food and Agriculture Organization/World Health Organization (FAO/WHO).

The purpose of this document is to reassess the existing exemption from the requirement of a tolerance for residues of gluconic acid and sodium salt as required under the Food Quality Protection Act (FQPA).

Executive Summary

This report evaluates gluconic acid and sodium salt, pesticide inert ingredients for which an exemption from the requirement of a tolerance exists for their residues when used in pesticide

formulations applied to growing crops only under 40 CFR §180.920 [formerly 40 CFR §180.1001(d)] as well as D-gluconic acid, monosodium salt, an ingredient in antimicrobial food-contact surface sanitizing solutions for which an exemption from the requirement of a tolerance exists for its residues under 49 CFR §180.940(b).

Gluconic acid and sodium salt is a term that includes gluconic acid (CAS Reg. No. 133-42-6), D-gluconic acid (CAS Reg. No. 526-95-4), sodium gluconate (CAS Reg. No. 527-07-1) and D-gluconic acid, sodium salt (CAS Reg. No. 14906-97-9). As food additives gluconic acid and its sodium salt have been evaluated by the Joint FAO/WHO Expert Committee on Food Additives (JECFA) which determined that these substances were of very low toxicity. In addition, these substances are considered to be Generally Recognized as Safe (GRAS) by the Food and Drug Administration when used as direct food additives.

Taking into consideration all available information on gluconic acid and sodium salt, including the categorization of these substances as Generally Recognized as Safe (GRAS) direct food additives by FDA and the determination by the Joint FAO/WHO Expert Committee on Food Additives (JECFA) that these substances are of very low toxicity, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposure to gluconic acid and sodium salt when considering dietary exposure and all other non-occupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemption from the requirement of a tolerance established for residues of gluconic acid and sodium salt in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCA.

I. Introduction

This report evaluates gluconic acid and sodium salt, a pesticide inert ingredient for which an exemption from the requirement of a tolerance exists for its residues when used in pesticide formulations applied to growing crops only under 40 CFR §180.920 [formerly 40 CFR §180.1001(d)] as well as D-gluconic acid, monosodium salt, an ingredient in antimicrobial food-contact surface sanitizing solutions for which an exemption from the requirement of a tolerance exists for its residues under 49 CFR §180.940(b).

Gluconic acid and sodium salt is a term that includes gluconic acid (CAS Reg. No. 133-42-6), D-gluconic acid (CAS Reg. No. 526-95-4), sodium gluconate (CAS Reg. No. 527-07-1) and D-gluconic acid, sodium salt (CAS Reg. No. 14906-97-9). In aqueous solutions, D-gluconic acid exists in an equilibrium with *gamma*- and *delta*-D-lactone and is sometimes referred to as D-glucono-*delta*-lactone. D-Glucono-*delta*-lactone is used as a sequestrant in the dairy industry to prevent “milk stone” and in breweries to prevent “beer stone” as well as being regarded by the Food and Drug Administration (FDA) as an affirmed generally recognized as safe (GRAS) direct food additive. Sodium gluconate is recognized by the FDA as a GRAS direct food additive as a sequestrant.

As food additives, gluconic acid and its sodium salt have been evaluated by the Joint FAO/WHO Expert Committee on Food Additives (JECFA), which determined that these substances were of very low toxicity and allocated an acceptable daily intake of “not specified.”

II. Use Information

Pesticides

The tolerance exemption for the inert ingredient gluconic acid and sodium salt is given in Table 1 below.

Table 1. Tolerance Exemption Being Reassessed in this Document				
Tolerance Exemption Expression	CAS Reg No.	40 CFR §	Use Pattern (Pesticidal)	List Classification
Gluconic acid and sodium salt	133-42-6 (gluconic acid)	180.920 ^{1/}	Sequestrant	3
	526-95-4 (D-gluconic acid)			3
	527-07-1 (sodium gluconate)			4B
	14906-97-9 (D-gluconic acid, sodium salt)			not listed
D-Gluconic acid, monosodium salt	527-07-1	180.940(b) ^{2/}	When ready for use, the end-use concentration is not to exceed 760 ppm	4B

1. Residues listed in formerly 40 CFR§ 180.100(d)] are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to growing crops only.

2. Residues listed in 40 CFR §180.940(b) are exempted from the requirement of a tolerance when used as ingredients in an antimicrobial pesticide formulation applied to: Dairy processing equipment, and food-processing equipment and utensils.

Other Uses

Table 2 below summarizes the FDA approved food additive uses for D-gluconic acid (as D-glucono-delta-lactone) and sodium gluconate.

Table 2. FDA Approved Food Additive Uses		
Chemical	21 CFR §	Uses
D-Glucono-delta-lactone	133.129	Curding agent in dry curd cottage cheese
	155.120	Media agent component in canned green beans and canned wax beans
	184.1318	Affirmed GRAS direct food additive for use in curing and pickling agent, leavening agent, pH control agent and sequestrant
Sodium Gluconate	182.6757	GRAS direct food additive–sequestrant

Gluconic acid and sodium salt are used as chelating agents; gluconic acid is commercially available as a 50% aqueous solution (TOXNET, 2005).

III. Physical and Chemical Properties

Appendix A lists some of the physical and chemical characteristics of gluconic acid and sodium salt.

IV. Hazard Assessment

A. Hazard Profile

Gluconic acid and its sodium salt have been evaluated by the Joint FAO/WHO Expert Committee on Food Additives (JECFA), which determined that these substances were of very low toxicity and allocated an acceptable daily intake of “not specified”¹ (JECFA, 1999).

B. Toxicological Data

Toxicological studies considered by JECFA in their evaluation of gluconic acid and its sodium salt included acute oral toxicity studies in the rat, mouse, rabbit and hamster with LD50

¹ ADI “not specified” is used to refer to a food substance of very low toxicity, which, on the basis of the available data (chemical, biochemical, toxicological, and other) and the total dietary intake of the substance arising from its use at the levels necessary to achieve the desired effect and from its acceptable background levels in food, does not, in the opinion of the Committee, represent a hazard to health. For that reason, and for reasons stated in individual evaluations, the establishment of an ADI expressed in numerical form is not deemed necessary. An additive meeting this criterion must be used within the bounds of good manufacturing practice, i.e., it should be technologically efficacious and should be used at the lowest level necessary to achieve this effect, it should not conceal food of inferior quality or adulterated food, and it should not create a nutritional imbalance.

values ranging from >2000 mg/kg to 7850 mg/kg. In various subchronic, chronic, developmental and reproductive studies evaluated by JECFA, no observable adverse effects were noted at limit dose levels (i.e., >1000mg/kg/day) or at the highest doses tested and these substances were negative in a number of bacterial reverse mutation assays (JECFA, 1999).

C. Special Considerations for Infants and Children

At this time, there is no concern for potential sensitivity to infants and children resulting from exposures to gluconic acid and sodium gluconate. In its evaluation of gluconic acid and sodium gluconate, JECFA reported no quantitative or qualitative evidence of increased susceptibility following the prenatal exposure to mice, rats, hamsters and rabbits in developmental toxicity studies (JECFA, 1999) at doses ranging up to 780 mg/kg/day (the highest dose tested). A safety factor analysis has not been used to assess the risk. For these reasons the additional tenfold safety factor for the protection of infants and children is unnecessary.

V. Exposure Assessment

Gluconic acid and sodium salt are of low toxicity to humans, and there is no reason to expect that reasonable use will constitute any significant hazard. Therefore, neither a qualitative or quantitative screening-level exposure assessment has been conducted.

VI. Aggregate Exposures

In examining aggregate exposure, FFDCA section 408 directs EPA to consider available information concerning exposures from the pesticide residue in food and all other non-occupational exposures, including drinking water from ground water or surface water and exposure through pesticide use in gardens, lawns, or buildings (residential and other indoor uses).

For gluconic acid and sodium salt, a qualitative assessment for all pathways of human exposure (food, drinking water, and residential) is appropriate given its very low toxicity.

VII. Cumulative Exposure

Section 408(b)(2)(D)(v) of the FFDCA requires that, when considering whether to establish, modify, or revoke a tolerance, the Agency consider "available information" concerning the cumulative effects of a particular pesticide's residues and "other substances that have a common mechanism of toxicity."

EPA does not have, at this time, available data to determine whether gluconic acid and sodium salt have a common mechanism of toxicity with other substances. Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding as to gluconic acid and sodium salt and any other substances and these materials do not appear to produce a toxic

metabolite produced by other substances. For the purposes of this tolerance action, therefore, EPA has not assumed that gluconic acid and sodium salt have a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA's Office of Pesticide Programs concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at <http://www.epa.gov/pesticides/cumulative/>.

VIII. Environmental Fate Characterization/Drinking Water Considerations

Based on modeling information, gluconic acid and sodium salt would undergo rapid biodegradation (hours to days) and would not be expected to be present in drinking water sources (EPI Suite, 2004). The estimated chemical fate properties of gluconic acid and sodium salt are given in Appendix B.

IX. Human Health Risk Characterization

Taking into consideration all available information on gluconic acid and sodium salt, including the categorization of these substance as Generally Recognized as Safe (GRAS) direct food additives by FDA and the determination by the Joint FAO/WHO Expert Committee on Food Additives (JEFCA) that these substances are of very low toxicity, it has been determined that there is a reasonable certainty that no harm to any population subgroup will result from aggregate exposures to gluconic acid and sodium salt when considering dietary exposure and all other non-occupational sources of pesticide exposure for which there is reliable information. Therefore, it is recommended that the exemptions from the requirement of a tolerance established for residues of gluconic acid and sodium salt in/on raw agricultural commodities can be considered reassessed as safe under section 408(q) of the FFDCA.

X. Ecotoxicity and Ecological Risk Characterization

There are no available aquatic toxicity studies on gluconic acid and sodium salt (ECOTOX, 2002), however, based on estimates of toxicity using physical and chemical property data, gluconic acid and sodium salt would be of low concern for toxicity to fish, algae, and aquatic invertebrates as well as terrestrial/benthic organisms (ECOSAR, 2000). The estimates of ecotoxicity of gluconic acid and sodium salt are given in Appendix C.

References:

ChemIDplus. 2005. ChemIDplus Advanced. U.S. National Library of Medicine. National Institutes of Health. Department of Health and Human Services. Online Search Database <http://chem.sis.nlm.nih.gov/chemidplus/>
Search term: Gluconic acid, sodium gluconate (February 4, 2005)

ECOSAR. 2000. Ecological Structure Activity Relationships Version 0.99g. Environmental Protection Agency. <http://www.epa.gov/oppt/newchems/21ecosar.htm>

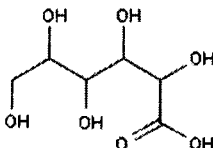
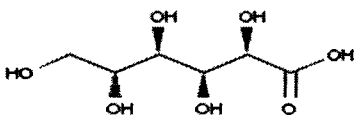
ECOTOX. 2002. U.S. Environmental Protection Agency. 2002. ECOTOX User Guide: ECOTOXicology Database System. Version 3.0. <http://www.epa.gov/ecotox/>
Search terms: CAS Reg Nos:133-42-6, 526, 95-4, 527-07-1, 14906-97-9 (February 4, 2005)

EPI Suite. 2004. Estimation Programs Interface Suite Version 3.12 (August 17, 2004). Environmental Protection Agency. <http://www.epa.gov/opptintr/exposure/docs/episuite.htm>

JECFA. 1999. Joint FAO/WHO Expert Committee on Food Additives. Safety Evaluation of Certain Food Additives: Glucono-delta-Lactone and the Calcium, Magnesium, Potassium, and Sodium Salts of Gluconic Acid. WHO Food Additive Series Vol. 42 pp 203-212. World Health Organization, Geneva. <http://www.inchem.org/documents/jecfa/jecmono/v042je12.htm>

TOXNET 2005. Hazardous Substance Data Bank (HSDB). On-line Scientific Search Engine, National Library of Medicine, National Institute of Health. <http://www.toxnet.nlm.nih.gov>.
Search term: Gluconic acid , sodium gluconate

Appendix A

Physical and Chemical Properties of Gluconic acid and Sodium Salt Measure (M) or Estimated (E)		
Parameter	Value	Source
Gluconic Acid (CAS Reg. No. 133-42-6)		
Structure		ChemIDplus, 2005
Molecular Weight	196.154	ChemIDplus, 2005
Water Solubility	3.16×10^5 mg/L at 25°C (E)	EPISuite, 2004
Melting Point	131° C (M)	EPISuite, 2004
Henry's Law Constant	4.74×10^{-13} atm-m ³ /mole @25°C (E)	EPISuite, 2004
Vapor Pressure	8.17×10^{-10} mmHg @25°C (E)	EPISuite, 2004
Octanol/Water Partition Coefficient	log P = -1.870 (E)	EPISuite, 2004
D-Gluconic acid (CAS Reg. No 526-95-4)		
Structure		ChemIDplus, 2005
Molecular Weight	196.154	ChemIDplus, 2005
Water Solubility	16×10^5 mg/L at 25°C (M)	ChemIDplus, 2005
Melting Point	131 ° C (E)	ChemIDplus, 2005
Henry's Law Constant	4.74×10^{-13} atm-m ³ /mole @25°C (E)	ChemIDplus, 2005
Vapor Pressure	3.72×10^{-10} mmHg @25°C (E)	ChemIDplus, 2005

Physical and Chemical Properties of Gluconic acid and Sodium Salt Measure (M) or Estimated (E)		
Parameter	Value	Source
Octanol/Water Partition Coefficient	log P = -1.870 (E)	ChemIDplus, 2005
Sodium Gluconate (CAS Reg. No. 527-07-1)		
Structure		ChemIDplus, 2005
Molecular Weight	218.136	ChemIDplus, 2005
Water Solubility	5.90 x 10 ⁵ mg/L at 25°C (M)	ChemIDplus, 2005
Melting Point	265.41° C (M)	EPISuite, 2004
Henry's Law Constant	4.76 x 10 ⁻¹³² atm-m ³ /mole @25°C (E)	EPISuite, 2004
Vapor Pressure	7.23 x 10 ⁻¹⁸ mmHg @25°C (E)	EPISuite, 2004
Octanol/Water Partition Coefficient	log P =-5.990 (E)	ChemIDplus, 2005
D-Gluconic acid, sodium salt (CAS Reg. No. 14906-97-9)		
Structure		
Molecular Weight	218.14	EPISuite, 2004
Water Solubility	5.90 x 10 ⁵ mg/L at 25°C (E)	EPISuite, 2004
Melting Point	265.41 ° C (E)	EPISuite, 2004
Henry's Law Constant	4.76 x 10 ⁻¹³ atm-m ³ /mole @25°C (E)	EPISuite, 2004

Physical and Chemical Properties of Gluconic acid and Sodium Salt Measure (M) or Estimated (E)		
Parameter	Value	Source
Vapor Pressure	7.23×10^{-18} mmHg @25°C (E)	EPISuite, 2004
Octanol/Water Partition Coefficient	log P =-5.990 (E)	EPISuite, 2004

APPENDIX B

PHYSICAL AND CHEMICAL PROPERTIES OF SODIUM GLUCONATE AND GLUCONIC ACID

SMILES : [Na]OC(=O)C(O)C(O)C(O)C(O)CO

CHEM : Sodium gluconate

CAS NUM: 000527-07-1

MOL FOR: C6 H11 O7 Na1

MOL WT : 218.14

----- EPI SUMMARY (v3.12) -----

Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m³/mole) : -----

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = -5.99

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C): 613.05 (Adapted Stein & Brown method)

Melting Pt (deg C): 265.41 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 7.23E-018 (Modified Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 1e+006

log Kow used: -5.99 (estimated)

no-melting pt equation used

Water Sol (Exper. database match) = 5.9e+005 mg/L (25 deg C)

Exper. Ref: MERCK INDEX (1996)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1e+006 mg/L

Wat Sol (Exper. database match) = 590000.00

Exper. Ref: MERCK INDEX (1996)

ECOSAR Class Program (ECOSAR v0.99h):

Class(es) found:

Neutral Organics

Henry's Law Constant (25 deg C) [HENRYWIN v3.10]:

Bond Method : 4.76E-013 atm-m³/mole

Group Method: Incomplete

Henry's LC [VP/WSol estimate using EPI values]: 2.075E-024 atm-m³/mole

Probability of Rapid Biodegradation (BIOWIN v4.02):

Biowin1 (Linear Model) : 1.4373

Biowin2 (Non-Linear Model) : 0.9959

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 3.5170 (days-weeks)

Biowin4 (Primary Survey Model) : 4.1803 (days)

Readily Biodegradable Probability (MITI Model):

Biowin5 (MITI Linear Model) : 0.7156

Biowin6 (MITI Non-Linear Model): 0.7823

Ready Biodegradability Prediction: YES

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 38.1277 E-12 cm³/molecule-sec

Half-Life = 0.281 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 3.366 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 10

Log Koc: 1.000

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):

Log BCF = 0.500 (BCF = 3.162)

log Kow used: -1.87 (estimated)

Volatilization from Water:

Total removal: 1.85 percent

Total biodegradation: 0.09 percent

Total sludge adsorption: 1.75 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.863	6.73	1000
Water	40.4	208	1000
Soil	58.7	416	1000
Sediment	0.0698	1.87e+003	0

Persistence Time: 270 hr

SMILES : O=C(O)C(O)C(O)C(O)C(O)CO

CHEM : D-Gluconic acid

CAS NUM: 000526-95-4

MOL FOR: C6 H12 O7

MOL WT : 196.16

----- EPI SUMMARY (v3.12) -----

Physical Property Inputs:

Water Solubility (mg/L): -----
Vapor Pressure (mm Hg) : -----
Henry LC (atm-m³/mole) : -----
Log Kow (octanol-water): -----
Boiling Point (deg C) : -----
Melting Point (deg C) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = -1.87

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C): 417.09 (Adapted Stein & Brown method)

Melting Pt (deg C): 161.68 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 8.17E-010 (Modified Grain method)

MP (exp database): 131 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 1e+006

log Kow used: -1.87 (estimated)

no-melting pt equation used

Water Sol (Exper. database match) = 3.16e+005 mg/L (25 deg C)

Exper. Ref: MERCK INDEX (1996)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1e+006 mg/L

Wat Sol (Exper. database match) = 316000.00

Exper. Ref: MERCK INDEX (1996)

ECOSAR Class Program (ECOSAR v0.99h):

Class(es) found:

Neutral Organics-acid

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:

Bond Method : 4.74E-013 atm-m³/mole

Group Method: Incomplete

Henrys LC [VP/WSol estimate using EPI values]: 2.109E-016 atm-m³/mole

Probability of Rapid Biodegradation (BIOWIN v4.02):

Biowin1 (Linear Model) : 1.5205

Biowin2 (Non-Linear Model) : 0.9984

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 3.9301 (days)

Biowin4 (Primary Survey Model) : 4.5975 (hours-days)

Readily Biodegradable Probability (MITI Model):

Biowin5 (MITI Linear Model) : 0.9622

Biowin6 (MITI Non-Linear Model): 0.9547

Ready Biodegradability Prediction: YES

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 42.3224 E-12 cm³/molecule-sec

Half-Life = 0.253 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 3.033 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 10

Log Koc: 1.000

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):

Log BCF = 0.500 (BCF = 3.162)

log Kow used: -1.87 (estimated)

Volatilization from Water:

Henry LC: 4.74E-013 atm-m³/mole (estimated by Bond SAR Method)

Half-Life from Model River: 1.73E+009 hours (7.208E+007 days)

Half-Life from Model Lake : 1.887E+010 hours (7.864E+008 days)

Removal In Wastewater Treatment:

Total removal: 1.85 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.75 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00262	6.06	1000
Water	26.8	55.9	1000
Soil	73.2	112	1000
Sediment	0.0344	503	0

Persistence Time: 123 hr

SMILES : [Na]OC(=O)C(O)C(O)C(O)C(O)CO

CHEM : Sodium gluconate

CAS NUM: 000527-07-1

MOL FOR: C6 H11 O7 Na1

MOL WT : 218.14

----- EPI SUMMARY (v3.12) -----

Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m³/mole) : -----

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = -5.99

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C): 613.05 (Adapted Stein & Brown method)

Melting Pt (deg C): 265.41 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 7.23E-018 (Modified Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 1e+006

log Kow used: -5.99 (estimated)

no-melting pt equation used

Water Sol (Exper. database match) = 5.9e+005 mg/L (25 deg C)

Exper. Ref: MERCK INDEX (1996)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1e+006 mg/L

Wat Sol (Exper. database match) = 590000.00

Exper. Ref: MERCK INDEX (1996)

ECOSAR Class Program (ECOSAR v0.99h):

Class(es) found:

Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:

Bond Method : 4.76E-013 atm-m3/mole

Group Method: Incomplete

Henrys LC [VP/WSol estimate using EPI values]: 2.075E-024 atm-m3/mole

Probability of Rapid Biodegradation (BIOWIN v4.02):

Biowin1 (Linear Model) : 1.4373

Biowin2 (Non-Linear Model) : 0.9959

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 3.5170 (days-weeks)

Biowin4 (Primary Survey Model) : 4.1803 (days)

Readily Biodegradable Probability (MITI Model):

Biowin5 (MITI Linear Model) : 0.7156

Biowin6 (MITI Non-Linear Model): 0.7823

Ready Biodegradability Prediction: YES

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 38.1277 E-12 cm³/molecule-sec

Half-Life = 0.281 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 3.366 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 10

Log Koc: 1.000

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):

Log BCF = 0.500 (BCF = 3.162)

log Kow used: -1.87 (estimated)

Volatilization from Water:

Henry LC: 4.76E-013 atm-m³/mole (estimated by Bond SAR Method)

Half-Life from Model River: 1.817E+009 hours (7.569E+007 days)

Half-Life from Model Lake : 1.982E+010 hours (8.258E+008 days)

Removal In Wastewater Treatment:

Total removal: 1.85 percent

Total biodegradation: 0.09 percent

Total sludge adsorption: 1.75 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount	Half-Life	Emissions
	(percent)	(hr)	(kg/hr)
Air	0.863	6.73	1000
Water	40.4	208	1000

Soil	58.7	416	1000
Sediment	0.0698	1.87e+003	0

Persistence Time: 270 hr

APPENDIX C

ECOTOXICITY OF GLUCONIC ACID AND SODIUM GLUCONATE

SMILES : O=C(O)C(O)C(O)C(O)C(O)CO

CHEM : D-Gluconic acid

CAS Num: 000526-95-4

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C6 H12 O7

MOL WT : 196.16

Log Kow: -1.87 (KowWin estimate)

Melt Pt:

Wat Sol: 7.727E+006 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Neutral Organics-acid

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	6.19e+005

--> Acid moiety found: Predicted values multiplied by 10

Neutral Organics-acid	: Fish	96-hr	LC50	6.32e+006
Neutral Organics-acid	: Fish	14-day	LC50	6.19e+006
Neutral Organics-acid	: Daphnid	48-hr	LC50	5.18e+006
Neutral Organics-acid	: Green Algae	96-hr	EC50	2.59e+006
Neutral Organics-acid	: Fish	30-day	ChV	4.36e+005
Neutral Organics-acid	: Daphnid	16-day	EC50	48866.020
Neutral Organics-acid	: Green Algae	96-hr	ChV	27681.328

Neutral Organics-acid	: Fish (SW)	96-hr	LC50	2.23e+005
Neutral Organics-acid	: Mysid Shrimp	96-hr	LC50	2.88e+007 *
Neutral Organics-acid	: Earthworm	14-day	LC50	1.88e+005

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: 5.0

Green algal EC50 toxicity log Kow cutoff: 6.4

SMILES : [Na]OC(=O)C(O)C(O)C(O)C(O)CO

CHEM : Sodium gluconate

CAS Num: 000527-07-1

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C6 H11 O7 Na1

MOL WT : 218.14

Log Kow: -5.99 (KowWin estimate)

Melt Pt:

Wat Sol: 1.369E+011 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Neutral Organic SAR	: Fish	14-day	LC50	2.67e+009

(Baseline Toxicity)

Neutral Organics	: Fish	96-hr	LC50	5.24e+009
Neutral Organics	: Fish	14-day	LC50	2.67e+009
Neutral Organics	: Daphnid	48-hr	LC50	3.23e+009
Neutral Organics	: Green Algae	96-hr	EC50	1.28e+009
Neutral Organics	: Fish	30-day	ChV	1.86e+008
Neutral Organics	: Daphnid	16-day	EC50	5.03e+006
Neutral Organics	: Green Algae	96-hr	ChV	1.26e+006
Neutral Organics	: Fish (SW)	96-hr	LC50	2.52e+007
Neutral Organics	: Mysid Shrimp	96-hr	LC50	4.53e+011 *
Neutral Organics	: Earthworm	14-day	LC50	3.88e+005

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: 5.0

Green algal EC50 toxicity log Kow cutoff: 6.4

Chronic toxicity log Kow cutoff: 8.0

MW cutoff: 1000