

December 17, 2002

TEST PLAN FOR CARBAMATE HYDROCHLORIDE

Carbamate Hydrochloride CAS No. 65206-90-8	Data Available	Data Acceptable	Testing Required
Study	Y/N	Y/N	Y/N
PHYSICAL/CHEMICAL CHARACTERISTICS			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
ENVIRONMENTAL FATE			
Photodegradation	Y	Y	N
Stability in Water	Y	Y	N
Transport (Fugacity)	Y	Y	N
Biodegradation	Y	Y	N
ECOTOXICITY			
Acute Toxicity to Fish	Y	N	Y
Acute Toxicity to Invertebrates	Y	N	Y
Acute Toxicity to Aquatic Plants	Y	N	Y
MAMMALIAN TOXICITY			
Acute Toxicity	Y	Y	N
Repeated Dose Toxicity	N/A	N/A	N/A
Developmental Toxicity	N	N	Y
Reproductive Toxicity	N/A	N/A	N/A
Genetic Toxicity Gene Mutations	N	N	Y
Genetic Toxicity Chromosomal Aberrations	N	N	Y
Y = Yes N= No N/A = Not Applicable			

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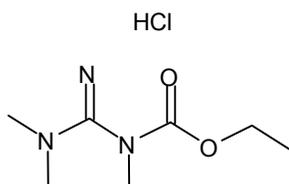
Existing published and unpublished data were collected and scientifically evaluated to determine the best possible study or studies to be summarized for each required endpoint. In the spirit of this voluntary program, other data of equal or lesser quality are not summarized, but are listed as related references at the end of each appropriate section, with a statement to reflect the reason why these studies were not summarized.

1.0 Substance Information

CAS Number: 65206-90-8

Chemical Name: Carbamate hydrochloride

Structural Formula:



Other Names: Carbamic acid, (aminoiminomethyl)methyl-, dimethyl deriv., ethyl ester monohydrochloride

F-3455.HCl

Exposure Limits: No Data.

2.0 Physical – Chemical Properties

2.1 Melting/Freezing Point:

Value: F3455.HCl: No Data
Product as shipped: -49.4°C (Freezing Point)

Decomposition: No Data

Pressure: No Data

Method: No Data

GLP: Unknown

Reference: DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).

Reliability: Not assignable because limited study information was available.

Additional References for Boiling Point: None Found.

2.2 Boiling Point:

Value: F3455.HCl: Not applicable

Product as shipped: 105°C
Decomposition: No Data
Pressure: No Data
Method: No Data
GLP: Unknown
Reference: DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability: Not assignable because limited study information was available.

Additional References for Boiling Point: None Found.

2.3 Density:

Value: F3455.HCl: Not applicable
Product as shipped: 69.7 lb/ft³
Temperature: 23°C
Method: No Data
GLP: Unknown
Results: No additional data.
Reference: DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability: Not assignable because limited study information was available.

Additional References for Density: None Found.

2.4 Vapor Pressure:

Value: F3455.HCl: Not applicable
Product as shipped: 18 mm Hg
Temperature: 21°C
Decomposition: No Data
Method: No Data
GLP: Unknown
Reference: DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability: Not assignable because limited study information was available.

Additional References for Vapor Pressure: None Found.

2.5 Partition Coefficient (log Kow):

Value: F-3455.HCl: -0.07
Temperature: 25°C

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Method: Modeled. KOWWIN, v. 1.66, module of EPIWINN 3.05 (Syracuse Research Corporation).
KOWWIN uses “fragment constant” methodologies to predict log P.
GLP: Not applicable
Reference: Meylan, W. M. and P. H. Howard (1995). J. Pharm. Sci., 84:83-92.
Reliability: Estimated based on an accepted model.

Additional References for Partition Coefficient (log Kow): None Found.

2.6 Water Solubility:

Value: F3455.HCl: At least 50%
Product as shipped: Infinite
Temperature: No Data
pH/pKa: No Data
Method: No Data
GLP: Unknown
Reference: DuPont Co. (2000). Unpublished Data.
Reliability: Not assignable because limited study information was available.

Additional References for Water Solubility: None Found.

2.7 Flash Point:

Value: F3455.HCl: Not applicable
Product as shipped: 60°C
Method: TCC
GLP: Unknown
Reference: DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability: Not assignable because limited study information was available.

Additional References for Flash Point: None Found.

2.8 Flammability: No Data.

3.0 Environmental Fate

3.1 Photodegradation:

Concentration: No Data

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Temperature: No Data
Direct Photolysis: Inspection of F-3455.HCl indicates that it may be subject to aquatic photodegradation.
Indirect Photolysis: No Data
Breakdown: No Data
Products:
Method: Inspection of chemical structure
GLP: Not Applicable
Reference: Harris, J. C. (1990). Rate of Aqueous Photolysis, Chapter 8 In Lyman, W. J. et al. (eds.). Handbook of Chemical Property Estimation Methods, American Chemical Society, Washington, DC.
Reliability: Estimate based on known qualitative structure-activity relationships.

Additional References for Photodegradation: None Found.

3.2 Stability in Water:

Concentration: No Data
Half-life: Hydrolyses very slowly (> 10 years at pH 7) in water.
% Hydrolyzed: No Data
Method: Modeled. HYDROWIN, v. 1.67 module of EPIWINN v3.05 (Syracuse Research Corporation). HYDROWIN estimates aqueous hydrolysis rate constants for the following chemical classes: esters, carbamates, epoxides, halomethanes and selected alkyl halides. HYDROWIN estimates acid- and base-catalyzed rate constants; it does NOT estimate neutral hydrolysis rate constants. The prediction methodology was developed for the U.S. Environmental Protection Agency and is outlined in Mill et al., 1987.
GLP: Not Applicable
Reference: Mill, T. et al. (1987). "Environmental Fate and Exposure Studies Development of a PC-SAR for Hydrolysis: Esters, Alkyl Halides and Epoxides" EPA Contract No. 68-02-4254, SRI International Menlo Park, CA.
Reliability: Estimate based on an accepted model.

Additional References for Stability in Water: None Found.

3.3 Transport (Fugacity):

Media: For F-3455.HCl
Air, Water, Soil, and Sediments

	Compartment	% of total distribution	½ life (hours) (advection + reaction)
	Air	0.005	15.1
	Water	45	360
	Soil	54.9	720
	Sediment	0.08	3240
Adsorption Coefficient:	Log K _{oc} = 0.349		
Desorption:	No Data		
Volatility:	Henry's Law Constant = 1.53×10^{-10} atm-m ² /mole		
Method:	Modeled, using 50% (w/v) water solubility value.		

Henry's Law Constant - HENRYWINN v. 3.10 module of EPIWINN v3.05 (Syracuse Research Corporation). Henry's Law Constant (HLC) is estimated by two separate methods that yield two separate estimates. The first method is the bond contribution method and the second is the group contribution method. The bond contribution method is able to estimate many more types of structures; however, the group method estimate is usually preferred (but not always) when all fragment values are available.

Log K_{oc} – Calculated from log K_{ow} by the Mackay Level III fugacity model incorporated into EPIWINN v3.05 (Syracuse Research Corporation).

Environmental Distribution - Mackay Level III fugacity model, in EPIWINN v3.05 (Syracuse Research Corporation). Emissions (1000 kg/hr) to air, water, and soil compartments.

GLP: Not Applicable

Reference: HENRYWIN – Hine, J. and P. K. Mookerjee (1975). J. Org. Chem., 40(3):292-8 and Meylan, W. and P. H. Howard (1991). Environ. Toxicol. Chem., 10:1283-93.

Fugacity - The methodology and programming for the Level III fugacity model incorporated into EPIWIN v3.05 (Syracuse Research Corporation) were developed by Dr. Donald MacKay and coworkers and are detailed in: Mackay, D. (1991). Multimedia Environmental Models: The Fugacity Approach, pp. 67-183, Lewis Publishers, CRC Press.

Mackay, D. et al. (1996). Environ. Toxicol. Chem., 15(9):1618-1626.

Mackay, D. et al. (1996). Environ. Toxicol. Chem., 15(9):1627-1637.

Reliability: Estimated values based on accepted model.

Additional References for Transport (Fugacity): None Found.

3.4 Biodegradation:

Value: Estimated half-life: 15 days, estimated to be readily biodegradable

Ultimate
Biodegradation
Timeframe: Weeks
Breakdown: No Data

Products:
Method: Modeled. BIOWIN, v. 4.0 module of EPINWINN v3.05 (Syracuse Research Corporation). BIOWIN estimates the probability for the rapid aerobic biodegradation of an organic chemical in the presence of mixed populations of environmental microorganisms. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

GLP: Not applicable

Reference: Boethling, R. S. et al. (1994). Environ. Sci. Technol., 28:459-65.
Howard, P. H. et al. (1992). Environ. Toxicol. Chem., 11:593-603.
Howard, P. H. et al. (1987). Environ. Toxicol. Chem., 6:1-10.
Tunkel, J. et al. (2000). "Predicting Ready Biodegradability in the MITI Test" Environ. Toxicol. Chem., accepted for publication.

Reliability: Estimated value based on accepted model.

Additional References for Biodegradation: None Found.

3.5 Bioconcentration:

Value: BCF = 3.162

Method: Modeled. BCFWIN v. 2.4 module of EPINWINN v3.05 (Syracuse Research Corporation). BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow) with correction factors based on molecular fragments.

GLP: Not applicable

Reference: "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997; prepared for:

Robert S. Boethling, EPA-OPPT, Washington, DC; Contract No. 68-D5-0012; prepared by: William M. Meylan, Philip H. Howard, Dallas Aronson, Heather Printup and Sybil Gouchie; Syracuse Research Corp.

Reliability: Estimated value based on accepted model.

Additional References for Bioconcentration: None Found.

4.0 Ecotoxicity

4.1 Acute Toxicity to Fish:

Type: 96-hour LC₅₀
Species: Fish
Value: 11,334 mg/L (log₁₀ Kow of -0.07)
Method: Modeled
GLP: Not Applicable
Test Substance: F3455.HCl
Results: No additional data.
Reference: Meylan, W. M. and P. H. Howard (1999). User's Guide for the ECOSAR Class Program, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).
Reliability: Estimated value based on accepted model.

Additional References for Acute Toxicity to Fish: None Found.

4.2 Acute Toxicity to Invertebrates:

Type: 48-hour EC₅₀
Species: Daphnid
Value: 10,527 mg/L (log₁₀ Kow of -0.07)
Method: Modeled
GLP: Not Applicable
Test Substance: F3455.HCl
Results: No additional data.
Reference: Meylan, W. M. and P. H. Howard (1999). User's Guide for the ECOSAR Class Program, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).

Reliability: Estimated value based on accepted model.

Additional References for Acute Toxicity to Invertebrates: None Found.

4.3 Acute Toxicity to Aquatic Plants:

Type: 96-hour EC₅₀
Species: Green algae
Value: 5842 mg/L (log₁₀ Kow of -0.07)
Method: Modeled
GLP: Not Applicable
Test Substance: F3455.HCl
Results: No additional data.
Reference: Meylan, W. M. and P. H. Howard (1999). User's Guide for the ECOSAR Class Program, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).
Reliability: Estimated value based on accepted model.

Additional References for Acute Toxicity to Aquatic Plants: None Found.

5.0 Mammalian Toxicity

5.1 Acute Toxicity:

Type: Oral ALD
Species/Strain: Rats/ChR-CD
Value: > 11,000 mg/kg
Method: No specific test guideline was reported; however, a scientifically defensible approach was used to conduct the study.

The test material, in original form, or as a solution in water, was administered to young adult male rats in single doses via intragastric intubation. Dose levels of 670, 1000, 1500, 2250, 3400, 5000, 7500, and 11,000 mg/kg were tested. One male rat was tested at each dose level. Survivors were sacrificed 13 or 14 days after dosing without pathological examinations.

GLP: No
Test Substance: Product as shipped (which contains 42% F3455.HCl)
Results: No mortality was observed. Lethargy was observed on the day of dosing at 7500 and 11,000 mg/kg. Slight initial

weight loss was evident at 670, 1500, 3400, 7500, and 11,000 mg/kg.
Reference: DuPont Co. (1974). Unpublished Data, Haskell Laboratory Report No. 70-74 "Acute Oral Test" (February 13).
Reliability: High because a scientifically defensible or guideline method was used.

Additional References for Acute Oral Toxicity: None Found.

Type: Inhalation Toxicity: No Data.

Type: Dermal Toxicity: No Data

Type: Dermal Irritation: No Data.

Type: Dermal Sensitization: No Data.

Type: Eye Irritation: No Data.

5.2 Repeated Dose Toxicity: No Data. Not a required endpoint.

5.3 Developmental Toxicity: No Data.

5.4 Reproductive Toxicity: No Data. Not a required endpoint.

5.5 Genetic Toxicity:

Type: *In vitro* Genetic Toxicity Studies: No Data.

Type: *In vivo* Genetic Toxicity Studies: No Data.