Supporting Documents for Initial Risk-Based Prioritization of High Production Volume Chemicals

Sponsored Chemical 3-Methyl benzonitrile (CASRN 620-22-4) (9th CI and CA Index Name: Benzonitrile, 3-methyl-)

Supporting Chemical Benzonitrile (CASRN 100-47-0)

Contents:

- Page 2: Background
- Page 4: Screening-Level Risk Characterization: September 2008
- Page 7: Screening-Level Hazard Characterization: September 2008
- Page 14: Screening-Level Exposure Characterization: September 2008

BACKGROUND

Screening-level hazard, exposure and risk characterizations for high production volume chemicals (HPV) are important contributions to the chemicals cooperation work being done in North America¹ through the EPA Chemical Assessment and Management Program (ChAMP)². These screening-level characterizations are developed by EPA for individual chemicals or chemical categories to support initial Risk-Based Prioritizations (RBPs) for HPV chemicals. These screening-level characterizations are technical documents intended primarily to inform the Agency's internal decision-making process. Accordingly, they are written for assessment professionals and assume a degree of technical understanding. Each of the support documents is described below.

The Risk-Based Prioritizations are found in an accompanying document and are written for a general audience. They present EPA's initial thinking regarding the potential risks presented by these chemicals and future possible actions that may be needed.

Hazard Characterizations for HPV Chemicals

EPA's screening-level hazard characterizations are based primarily on the review of the summaries of studies and other information submitted by the chemical sponsor(s) under the HPV Challenge Program³. These studies included in the scope of the HPV Challenge comprise the Screening Information Data Set (SIDS) of the Organization for Economic Cooperation and Development (OECD)⁴, an internationally recognized battery of tests that provides the basic data necessary to make an initial evaluation of a chemical's hazards and fate. In preparing the initial hazard characterizations, EPA also consulted a variety of reliable sources⁵ for additional relevant information and considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of an HPV submission, EPA also searched publicly available databases⁶ for information entered from one year prior to the HPV submission through May 2008. The screening-level hazard characterization is performed according to established EPA guidance⁷. A more detailed description of the hazard characterization process is available on the EPA website⁸.

With respect to chemicals for which internationally-accepted OECD SIDS Initial Assessment Profiles (SIAP) and Initial Assessment Reports (SIAR) were available, EPA did not generate its own screening-level hazard characterization, but did check for and incorporate updated information in the risk characterization.

Exposure Characterizations for HPV Chemicals

EPA recently received exposure-related data on chemicals submitted in accordance with the requirements of Inventory Update Reporting (IUR)⁹. The 2006 IUR submissions pertain to chemicals manufactured in

¹ U.S. EPA – U.S. Commitments to North American Chemicals Cooperation: http://www.epa.gov/hpv/pubs/general/sppframework.htm.

² U.S. EPA – ChAMP information: http://www.epa.gov/champ/.

³ U.S. EPA – HPV Challenge Program information: http://www.epa.gov/hpv.

⁴ U.S. EPA – Technical Guidance Document, OECD SIDS Manual Sections 3.4 and 3.5: http://www.epa.gov/chemrtk/pubs/general/sidsappb.htm.

⁵ U.S. EPA – Public Database Hazard Information: http://www.epa.gov/hpvis/hazardinfo.htm.

⁶ U.S. EPA – Public Database Update Information: http://www.epa.gov/chemrtk/hpvis/updateinfo.htm.

⁷ U.S. EPA – Risk Assessment Guidelines: http://cfpub.epa.gov/ncea/raf/rafguid.cfm.

⁸ U.S. EPA – About HPV Chemical Hazard Characterizations: http://www.epa.gov/hpvis/abouthc.htm.

⁹ U.S. EPA – Basic IUR Information: http://www.epa.gov/opptintr/iur/pubs/guidance/basic-information.htm.

(including imported into) the U.S. during calendar year 2005 in quantities of 25,000 pounds or more at a single site. The reports include the identity, the quantity, and the physical form of the chemical manufactured or imported, and the number of workers reasonably likely to be exposed during manufacture of the chemical. For chemicals manufactured or imported in quantities of 300,000 pounds or more at a single site, additional reported information includes: the industrial processing and uses of the chemical; the number of industrial processing sites and workers reasonably likely to be exposed to the chemical at those sites; the consumer and commercial uses of the chemical; and an indication whether the chemical was used in products intended for use by children under 14 years of age.

EPA's screening-level exposure characterizations are based largely on the information submitted under the IUR reporting, although other exposure information submitted to the Agency (for example, in HPV submissions) or readily available through a limited set of publicly accessible databases¹⁰ was also considered. The screening-level exposure characterizations identify a potential (high, medium, or low) that each of five populations – the environment, the general population, workers, consumers, and children – might be exposed to the chemical. In most cases, this potential doesn't address the quantity, frequency, or duration of exposure, but refers only to the likelihood that an exposure could occur.

In many instances EPA is not able to fully disclose to the public all the IUR exposure-related data reviewed or relied upon in the development of the screening-level documents because some of the material was claimed as confidential business information (CBI) when it was submitted to the Agency. These CBI claims do limit the Agency's ability to be completely transparent in presenting some underlying exposure and use data for chemicals in public documents. EPA does consider all data, including data considered to be CBI, in the screening-level exposure and risk characterization process, and endeavors whenever possible to broadly characterize supporting materials claimed as confidential in ways that do not disclose actual CBI.

Risk Characterizations for HPV Chemicals

EPA combines the information from the screening-level exposure characterization with the screening-level hazard characterization to develop a qualitative screening-level risk characterization, as described in the Agency's guidance on drafting risk characterizations¹¹. These screening-level risk characterizations are technical documents intended to support subsequent priority-setting decisions and actions by OPPT. The purpose of the qualitative screening-level risk characterization is two-fold: to support initial risk-based decisions to prioritize chemicals, identify potential concerns, and inform risk management options; and to identify data needs for individual chemicals or chemical categories.

These initial characterization and prioritization documents do not constitute a final Agency determination as to risk, nor do they determine whether sufficient data are available to characterize risk. Recommended actions reflect EPA's relative judgment regarding this chemical or chemical category in comparison with others evaluated under this program, as well as the uncertainties presented by gaps that may exist in the available data.

¹⁰ U.S. EPA – Summary of Public Databases Routinely Searched: http://www.epa.gov/chemrtk/hpvis/pubdtsum.htm.

¹¹ U.S. EPA – Risk Characterization Program: http://www.epa.gov/osa/spc/2riskchr.htm.

QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION OF HIGH PRODUCTION VOLUME CHEMICALS

SPONSORED CHEMICAL

3-Methyl Benzonitrile (CAS No. 620-22-4) [9th CI Name: Benzonitrile, 3-methyl-]

SUPPORTING CHEMICAL

Benzonitrile (CAS No. 100-47-0)

September 2008

Prepared by

Risk Assessment Division
Economics, Exposure and Technology Division
Office of Pollution Prevention and Toxics
Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, DC 20460-0001

QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION FOR 3-Methyl Benzonitrile (CAS No. 620-22-4)

1. Physical-Chemical Properties and Environmental Fate

3-Methylbenzonitrile is a clear, colorless liquid at room temperature. It is estimated to have moderate water solubility and vapor pressure. It has moderate mobility in soil and moderate volatility. 3-Methylbenzonitrile undergoes atmospheric photooxidation at a rate that is considered slow. No biodegradation or stability in water (hydrolysis) data for 3-methylbenzonitrile were submitted; however, EPA located ready biodegradability studies on related substances indicating that the substances were readily biodegradable. Based on this information and modeling, the environmental persistence of this substance is expected to be low (P1). An estimated BCF of 8 suggests that 3-methylbenzonitrile has a low bioaccumulation potential (B1).

2. Hazard Characterization

Aquatic Organism Toxicity. The acute aquatic toxicity of 3-methylbenzonitrile to fish, aquatic invertebrates and plants is expected to be low based on data for the supporting chemical benzonitrile (CAS No. 100-47-0).

Human Health Toxicity. The acute oral toxicity of 3-methylbenzonitrile is low. 3-Methylbenzonitrile is slightly irritating to rabbit skin and severely irritating to rabbit eyes. Repeated-dose and reproductive toxicity data were not required for the HPV Challenge Program because 3-methylbenzonitrile is a closed-system intermediate. 3-Methylbenzonitrile did not induce gene mutations.

3. Exposure Characterization

There are no 2006 Inventory Update Rule submissions for this chemical. Information submitted as part of the HPV Challenge Program indicates that this chemical is used as a process intermediate in the synthesis of a fungicide.

Potential for Exposures to Human and the Environment:

Based on information from the HPV Challenge Program and in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a low relative ranking for each of the potentially exposed groups, including workers, general population, consumers and children, and the environment. In 2007, the Agency reviewed the information in the HPV submission or test plan and determined that the HPV chemical satisfies the guidance to demonstrate that the chemical is a closed system intermediate. The chemical is manufactured and processed in systems that are expected to reduce the potential for worker exposure and environmental releases that could lead to other human and environmental exposure. The guidance for identifying this chemical substance as a closed-system intermediate was satisfied at all sites reporting this chemical in accordance with IUR requirements. No information on commercial/consumer uses were found in the IUR or other data sources.

4. Risk Characterization

The statements and rationale provided below are intended solely for the purpose of this screening-level and qualitative risk characterization and will be used for prioritizing substances for future work in the Chemical Assessment and Management Program (ChAMP).

Risk Statement and Rationale

The Agency has reviewed the information in the HPV submission or test plan and determined that the HPV chemical satisfies the guidance to demonstrate that the chemical is a closed system intermediate (CSI). 3-Methylbenzonitrile is manufactured and processed in closed systems that are expected to significantly reduce the potential for worker exposure and environmental releases that could lead to other human and environmental exposure. Therefore, there is a low concern for potential risks to aquatic organisms and the general population from environmental releases, and also to workers, consumers, and children.

SCREENING-LEVEL HAZARD CHARACTERIZATION OF HIGH PRODUCTION VOLUME CHEMICALS

SPONSORED CHEMICAL

3-Methyl Benzonitrile (CAS No. 620-22-4) [9th CI Name: Benzonitrile, 3-methyl-]

SUPPORTING CHEMICAL

Benzonitrile (CAS No. 100-47-0)

September 2008

Prepared by

Risk Assessment Division
Economics, Exposure and Technology Division
Office of Pollution Prevention and Toxics
Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, DC 20460-0001

SCREENING-LEVEL HAZARD CHARACTERIZATION 3-Methyl Benzonitrile (CAS No. 620-22-4)

Introduction

The sponsor, Syngenta Crop Protection, Inc., submitted a Test Plan and Robust Summaries to EPA for 3-methyl benzonitrile (CAS No. 620-22-4; 9th CI name: benzonitrile, 3-methyl-) on January 05, 2006. EPA posted the submission on the ChemRTK HPV Challenge Web site on February 22, 2006 (http://www.epa.gov/chemrtk/pubs/summaries/3methbnz/c16166tc.htm). EPA comments on the original submission were posted to the website on August 16, 2007. Public comments were also received and posted to the website.

This screening level hazard characterization is based primarily on the review of the test plan and robust summaries of studies submitted by the sponsor(s) under the HPV Challenge Program. In preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as any sponsors responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from 2004 to May 2008: the NLM databases (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. A summary table of SIDS endpoint data with the structure(s) of the sponsored chemical(s) is included in the appendix. The screening-level hazard characterization for environmental and human health effects is based largely on SIDS endpoints and is described according to established EPA or OECD effect level definitions and hazard assessment practices.

The sponsor proposed reduced health effects testing claiming that 3-methyl benzonitrile is a closed-system intermediate (CSI). EPA's evaluation of the original information indicated that the chemical meets the guidance to support the CSI claim for this chemical. 3-methyl benzonitrile is formed as an intermediate during the synthesis of isophthalonitrile (IPN) which is subsequently used on-site to produce the FIFRA regulated fungicide, Chlorothalonil. Transport of 3-methyl benzonitrile to other sites does not occur. Therefore, EPA has determined that the chemical qualifies for reduced testing and waiving of repeated-dose and reproductive toxicity testing for the purposes of the HPV Challenge Program.

EPA has identified that data for benzonitrile (CAS No. 100-47-0) can be used to address the ecotoxicity endpoints for the purposes of the HPV Challenge Program. Benzonitrile is structurally similar to 3-methyl benzonitrile and has similar physical-chemical properties.

Hazard Characterization

3-Methylbenzonitrile is a clear, colorless liquid at room temperature. It is estimated to have moderate water solubility and vapor pressure. It has moderate mobility in soil and moderate volatility. 3-Methylbenzonitrile undergoes atmospheric photooxidation at a rate that is considered slow. An estimated BCF of 8 suggests that 3-methylbenzonitrile has a low bioaccumulation potential (B1). No biodegradation or stability in water (hydrolysis) data for 3-methylbenzonitrile were submitted; however, EPA located ready biodegradability studies on related substances indicating that the substances were readily biodegradable. Based on this information and modeling, the environmental persistence of this substance is expected to be low (P1).

The acute aquatic toxicity of 3-methylbenzonitrile to fish, aquatic invertebrates and plants is expected to be low based on data for the supporting chemical benzonitrile (CAS No. 100-47-0).

The acute oral toxicity of 3-methylbenzonitrile is low. 3-Methylbenzonitrile is slightly irritating to rabbit skin and severely irritating to rabbit eyes. Repeated-dose and reproductive toxicity data were not required for the HPV Challenge Program because 3-methylbenzonitrile is a closed-system intermediate. 3-Methylbenzonitrile did not induce gene mutations.

Vapor pressure, water solubility, ready biodegradation, developmental toxicity, and chromosomal aberration assays were identified as data gaps under the HPV Challenge Program.

1. Physical-Chemical Properties and Environmental Fate

The physical-chemical properties of 3-methylbenzonitrile are summarized in Table 1a, while its environmental fate properties are given in Table 1b. The structure of the compound is provided in the Appendix.

Physical-Chemical Properties Characterization

3-Methylbenzonitrile is liquid that has moderate water solubility and moderate vapor pressure based on estimated values. Estimated values for vapor pressure and water solubility were provided by the sponsor for 3-methylbenzonitrile and used to characterize these endpoints. However, estimated values for these endpoints are not adequate for the HPV Challenge Program unless the solubility is <1 ppb and the vapor pressure is lower than 1×10^{-5} Pa.

Table 1a. Physical-Chemical Properties of 3-Methylbenzonitrile ¹		
Property	Value	
CAS No.	620-22-4	
Molecular Weight	117.15	
Physical State	Liquid	
Melting Point	-23°C (measured)	
Boiling Point	213°C (measured)	
Vapor Pressure	$0.187 \text{ mm Hg (estimated)}^2$	
Henry's Law Constant	4.8×10^{-5} atm-m ³ /mole (estimated) ²	
Water Solubility	$921.2 \text{ mg/L (estimated)}^2$	
Log K _{ow}	2.087 (estimated) ²	

¹Syngenta Crop Protection Inc. 2005. Robust Summary and Test Plan for 3-Methylbenzonitrile. http://www.epa.gov/chemrtk/pubs/summaries/3methbnz/c16166tc.htm.

Environmental Fate Characterization

3-Methylbenzonitrile is expected to partition primarily to soil and water according to the results of a Level III fugacity model that assumes equal emissions to air, water, and soil. 3-Methylbenzonitrile is expected to possess moderate mobility in soil. 3-Methylbenzonitrile undergoes atmospheric photooxidation with photochemically generated hydroxyl radicals at a rate that is considered slow. An estimated BCF of 8 suggests that 3-methylbenzonitrile has a low bioaccumulation potential (B1). No biodegradation or stability in water (hydrolysis) data for 3-methylbenzonitrile were submitted; however, EPA located ready biodegradability data for benzonitrile and 4-hydroxybenzonitrile indicating that they are both readily biodegradable. The combination of these measured values and modeling lead to the conclusion that the environmental persistence of 3-methylbenzonitrile will be low (P1). Measured ready biodegradation and hydrolysis data were not submitted and are therefore considered data gaps under the HPV Challenge Program.

²US EPA. 2008. Estimation Programs Interface Suite[™] for Microsoft® Windows, v 3.20. United States Environmental Protection Agency, Washington, DC, USA. http://www.epa.gov/opptintr/exposure/pubs/episuite.htm.

U.S. Environmental Protection Agency Supporting Documents for Risk-Based Prioritization

Table 1b. Environmental Fate Characteristics of 3-Methylbenzonitrile ¹		
Property	Value	
Photodegradation Half-life	13.3 days (estimated)	
Biodegradation	Data Gap	
	Readily biodegradable based on analogs ² and modeling ³	
Hydrolysis Half-life	Data Gap	
Bioconcentration	$BCF = 8 \text{ (estimated)}^3$	
K _{oc}	2.17 (estimated) ³	
Fugacity	Air = 8.1%	
(Level III Model) ²	Water = 28.5%	
	Soil = 63.3%	
	Sediment = 0.1%	
Persistence ³	P1 (low)	
Bioaccumulation3	B1 (low)	

¹Syngenta Crop Protection Inc. 2005. Robust Summary and Test Plan for 3-Methylbenzonitrile. http://www.epa.gov/chemrtk/pubs/summaries/3methbnz/c16166tc.htm.

Conclusion: 3-Methylbenzonitrile is a clear, colorless liquid at room temperature. It is estimated to have moderate water solubility and vapor pressure. It has moderate mobility in soil and moderate volatility. 3-Methylbenzonitrile undergoes atmospheric photooxidation at a rate that is considered slow. No biodegradation or stability in water (hydrolysis) data for 3-methylbenzonitrile were submitted; however, EPA located ready biodegradability studies on related substances indicating that the substances were readily biodegradable. Based on this information and modeling, the environmental persistence of this substance is expected to be low (P1). An estimated BCF of 8 suggests that 3-methylbenzonitrile has a low bioaccumulation potential (B1).

2. Environmental Effects – Aquatic Toxicity

Acute toxicity to Fish

3-Methyl benzonitrile(CAS No. 620-22-4)

Acute toxicity to fish from 3-methyl benzonitrile was estimated using ECOSAR.

96-h $LC_{50} = 71.5 \text{ mg/L}$

Benzonitrile (CAS No. 100-47-0, Supporting Chemical)

Fish (several species) were exposed to benzonitrile in 16 studies reported in EPA's ECOTOX database.

 $96-h\ LC_{50} = 54 - 400\ mg/L$

Acute Toxicity to Aquatic Invertebrates

3-Methyl benzonitrile (CAS No. 620-22-4)

Acute toxicity to aquatic invertebrates from 3-methyl benzonitrile was estimated using ECOSAR. 48-h $LC_{50} = 77.1 \text{ mg/L}$

Benzonitrile (CAS No. 100-47-0, Supporting Chemical)

Water fleas (*Daphnia magna*) were exposed to benzonitrile in three studies reported in EPA's ECOTOX database. 24-h $EC_{50} = 30.9 - 200$ mg/L

²National Institute of Technology and Evaluation, Tokyo, Japan. 2002. Biodegradation and Bioconcentration of the Existing Chemical Substances under the Chemical Substances Control Law. CAS Numbers 100-47-0 and 767-00-0. http://www.safe.nite.go.jp/english/kizon/KIZON_start_hazkizon.html.

³US EPA. 2008. Estimation Programs Interface Suite[™] for Microsoft® Windows, v 3.20. United States Environmental Protection Agency, Washington, DC, USA. http://www.epa.gov/opptintr/exposure/pubs/episuite.htm.

³Federal Register. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) pp. 60194–60204.

U.S. Environmental Protection Agency Supporting Documents for Risk-Based Prioritization

Toxicity to Aquatic Plants

3-Methyl benzonitrile (CAS No. 620-22-4)

Toxicity to aquatic plants from 3-methyl benzonitrile was estimated using ECOSAR.

96-h EC_{50} (growth) = 48.4 mg/L

Benzonitrile (CAS No. 100-47-0, Supporting Chemical)

Aquatic plants (several species) were exposed to benzonitrile in 13 studies reported in EPA's ECOTOX database. 72-h EC_{50} (growth) = 30 mg/L

Conclusion: No adequate aquatic toxicity data were submitted for 3-methyl benzonitrile. Based on ECOSAR estimations for 3-methyl benzonitrile and available toxicity data for the supporting substance benzonitrile (CAS No. 100-47-0), the acute toxicity to fish and aquatic invertebrates and toxicity to aquatic plants is expected to be low.

3. Human Health Effects

Acute Oral Toxicity

Sprague-Dawley rats (sex, number not stated) were administered 3-methyl benzonitrile via gavage at 3000 mg/kg-bw/day (in tragarth) and observed for 7 days. No further details were provided in the summary. Although the sponsor rated the study invalid, the results indicate the potential acute toxicity of the test substance.

 $LD_{50} > 3000$ mg/kg-bw/day

Repeated-Dose Toxicity

No repeated-dose toxicity data were provided. EPA has determined that 3-methyl benzonitrile meets the guidance to support a CSI claim and has waived the requirement for repeated-dose toxicity testing for the purposes of the HPV Challenge Program.

Reproductive Toxicity

No reproductive toxicity data were submitted. EPA has determined that 3-methyl benzonitrile meets the guidance to support a CSI claim and has waived the requirement for reproductive toxicity testing for the purposes of the HPV Challenge Program.

Developmental Toxicity

No developmental toxicity test data were submitted. Data gap

Genetic Toxicity - Gene Mutations

In Vitro

In an NTP study, *Salmonella typhimurium* strains TA97, TA98, TA100 and TA1535 were exposed to 3-methyl benzonitrile up to 3333 μ g/plate in the presence and absence of metabolic activation. Positive and negative controls gave the appropriate response. Cytotoxicity was observed at concentrations \geq 1000 μ g/plate. No mutagenicity was observed

3-Methylbenzonitrile was not mutagenic in this assay.

Genetic Toxicity - Chromosomal Aberrations

No chromosomal aberration test data were submitted. Data gap

U.S. Environmental Protection Agency Supporting Documents for Risk-Based Prioritization

Additional Information

Skin Irritation

White rabbits (strain and number not specified) were administered 3-methyl benzonitrile dermally on to their backs on cotton pads saturated with the test substance. After 15 minutes, the pads were removed and the application area was washed with undiluted polyethylene glycol 400 (PEG 400) and then with a 50% solution of PEG 400. After 20 hours, the skin was not washed. Skin reactions were scored immediately after pad removal and after 1, 3, and 8 days until the skin changes had disappeared. At 15 minutes slight vascular injection and at 20 hours, significant vascular injection was seen. Although the sponsor rated the study invalid, the results do provide indication of the potential irritating properties of the test substance.

3-Methyl benzonitrile was slightly irritating to rabbit skin.

Eye Irritation

Rabbits (strain and number not specified) were instilled 3-methyl benzonitrile into the conjunctival sac and spread over the upper eye. The reactions were scored after 10 minutes, 1 and 24 hours, 3 and 8 days and until the signs of irritation disappeared. 3-Methyl benzonitrile caused necrosis to the rabbit eye. Although the sponsor rated the study invalid, the results do provide indication of the potential irritating properties of the test substance.

3-Methyl benzonitrile was severely irritating to rabbit eyes in this study.

Conclusion: The acute oral toxicity of 3-methylbenzonitrile is low. 3-Methylbenzonitrile is slightly irritating to rabbit skin and severely irritating to rabbit eyes. Repeated-dose and reproductive toxicity data were not required for the HPV Challenge Program because 3-methylbenzonitrile is a closed-system intermediate. 3-Methylbenzonitrile did not induce gene mutations.

APPENDIX

Summary Table of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program				
Endpoints	SPONSORED CHEMICAL 3-Methyl benzonitrile (620-22-4)	SUPPORTING CHEMICAL Benzonitrile (100-47-0)		
Structure	CN	CN		
Summary of Environmental Effects – Aquatic Toxicity Data				
Fish 96-h LC ₅₀ (mg/L)	71.5 (estimate)	54 – 400		
Aquatic Invertebrates 48-h EC ₅₀ (mg/L)	77.1 (estimate)	30.9 – 200 (24-h)		
Aquatic Plants 72-h EC ₅₀ (mg/L)	48.4 (96-h) (estimate)	30.0		
Summary of Human Health Data				
Acute Oral Toxicity LD ₅₀ (mg/kg-bw)	> 3000	*		
Repeated-Dose Toxicity NOAEL/LOAEL	Endpoint waived because the chemical is a closed system intermediate.	*		
Reproductive Toxicity NOAEL/LOAEL	Endpoint waived because the chemical is a closed system intermediate.	*		
Developmental Toxicity NOAEL/LOAEL	Data Gap	*		
Genetic Toxicity – Gene Mutation	Negative	*		
Genetic Toxicity – Chromosomal Aberrations	Data Gap	*		
Additional Information Skin Irritation Eye Irritation	Slightly irritating Severely irritating	**		

[—] indicates that endpoint was not addressed for this chemical; * indicates endpoint not necessary for supporting chemical; ** indicates endpoints that are not part of the base Screening Information Data Set (SIDS).

Screening Level Exposure Characterization for HPV Challenge Chemical

Benzonitrile, 3-methyl CAS # 620-22-4

September 2008

Prepared by

Exposure Assessment Branch
Chemical Engineering Branch
Economics, Exposure and Technology Division
Office of Pollution Prevention and Toxics
Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, DC 20460-0001

Screening Level Exposure Characterization Benzonitrile, 3-methyl (CAS # 620-22-4)

Non-CBI Executive Summary

There are no 2006 Inventory Update Rule submissions for this chemical.

Information submitted as part of the HPV Challenge Program indicates that this chemical is used as a process intermediate in the synthesis of a fungicide. 12

Potential for Exposures to Human and the Environment:

Based on information from the HPV Challenge Program and in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a low relative ranking for each of the potentially exposed groups, including workers, general population, consumers and children, and the environment. In 2007, the Agency reviewed the information in the HPV submission or test plan and determined that the HPV chemical satisfies the guidance to demonstrate that the chemical is a closed system intermediate. The chemical is manufactured and processed in systems that are expected to reduce the potential for worker exposure and environmental releases that could lead to other human and environmental exposure. No information on commercial/consumer uses were found in the IUR or other data sources.

¹² Syngenta Crop Protection, Inc. 2005. Robust Summary and Test Plan for 3-Methylbenzonitrile. http://www.epa.gov/chemrtk/pubs/summaries/3methbnz/c16166tc.htm.

¹³ USEPA, 2007. EPA Comments on Chemical RTK HPV Challenge Submission. Letter dated November, 2007. http://www.epa.gov/chemrtk/pubs/summaries/3methbnz/c16166ct.pdf. Accessed June 20, 2008.