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Provisional Peer-Reviewed Toxicity Values for

Pentamethyl dipropylenetriamine
(CASRN 3855-32-1)

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Questions regarding the contents of this document may be directed to the U.S. EPA Office of Research and Development's National Center for Environmental Assessment, Superfund Health Risk Technical Support Center (513-569-7300).

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COMMONLY USED ABBREVIATIONS

BMC	benchmark concentration
BMD	benchmark dose
BMCL	benchmark concentration lower bound 95% confidence interval
BMDL	benchmark dose lower bound 95% confidence interval
HEC	human equivalent concentration
HED	human equivalent dose
IUR	inhalation unit risk
LOAEL	lowest-observed-adverse-effect level
$LOAEL_{ADJ}$	LOAEL adjusted to continuous exposure duration
$LOAEL_{HEC}$	LOAEL adjusted for dosimetric differences across species to a human
NOAEL	no-observed-adverse-effect level
$NOAEL_{ADJ}$	NOAEL adjusted to continuous exposure duration
$NOAEL_{HEC}$	NOAEL adjusted for dosimetric differences across species to a human
NOEL	no-observed-effect level
OSF	oral slope factor
p-IUR	provisional inhalation unit risk
p-OSF	provisional oral slope factor
p-RfC	provisional reference concentration (inhalation)
p-RfD	provisional reference dose (oral)
POD	point of departure
RfC	reference concentration (inhalation)
RfD	reference dose (oral)
UF	uncertainty factor
UF_A	animal-to-human uncertainty factor
UF_C	composite uncertainty factor
UF_D	incomplete-to-complete database uncertainty factor
UF_H	interhuman uncertainty factor
UF_L	LOAEL-to-NOAEL uncertainty factor
UF_S	subchronic-to-chronic uncertainty factor
WOE	weight of evidence

PROVISIONAL PEER-REVIEWED TOXICITY VALUES FOR PENTAMETHYL DIPROPYLENETRIAMINE (CASRN 3855-32-1)

BACKGROUND

A Provisional Peer-Reviewed Toxicity Value (PPRTV) is defined as a toxicity value derived for use in the Superfund Program. PPRTVs are derived after a review of the relevant scientific literature using established Agency guidance on human health toxicity value derivations. All PPRTV assessments receive internal review by a standing panel of National Center for Environment Assessment (NCEA) scientists and an independent external peer review by three scientific experts.

The purpose of this document is to provide support for the hazard and dose-response assessment pertaining to chronic and subchronic exposures to substances of concern, to present the major conclusions reached in the hazard identification and derivation of the PPRTVs, and to characterize the overall confidence in these conclusions and toxicity values. It is not intended to be a comprehensive treatise on the chemical or toxicological nature of this substance.

The PPRTV review process provides needed toxicity values in a quick turnaround timeframe while maintaining scientific quality. PPRTV assessments are updated approximately on a 5-year cycle for new data or methodologies that might impact the toxicity values or characterization of potential for adverse human health effects and are revised as appropriate. It is important to utilize the PPRTV database (http://hhpprtv.ornl.gov) to obtain the current information available. When a final Integrated Risk Information System (IRIS) assessment is made publicly available on the Internet (www.epa.gov/iris), the respective PPRTVs are removed from the database.

DISCLAIMERS

The PPRTV document provides toxicity values and information about the adverse effects of the chemical and the evidence on which the value is based, including the strengths and limitations of the data. All users are advised to review the information provided in this document to ensure that the PPRTV used is appropriate for the types of exposures and circumstances at the site in question and the risk management decision that would be supported by the risk assessment.

Other U.S. Environmental Protection Agency (EPA) programs or external parties who may choose to use PPRTVs are advised that Superfund resources will not generally be used to respond to challenges, if any, of PPRTVs used in a context outside of the Superfund program.

QUESTIONS REGARDING PPRTVS

Questions regarding the contents and appropriate use of this PPRTV assessment should be directed to the EPA Office of Research and Development's National Center for Environmental Assessment, Superfund Health Risk Technical Support Center (513-569-7300).

INTRODUCTION

Pentamethyl dipropylenetriamine (systematic name 1,3-propanediamine, *N1*-[3-(dimethylamino)propyl]-*N1,N3*,*N3*-trimethyl-), CAS No. 3855-32-1, is an aliphatic amine used primarily as an ingredient in polyurethane foam resins. The chemical structure of pentamethyl dipropylenetriamine is given in Figure 1. Molecular weight was the only physicochemical property available for this chemical (see Table 1). No references relevant to the derivation of provisional toxicity values for pentamethyl dipropylenetriamine were found, and no chemicals were identified as possible surrogates.

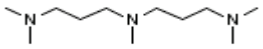

Figure 1. Pentamethyl Dipropylenetriamine Structure

Table 1. Physicochemical Properties Table (Pentamethyl Dipropylenetriamine CASRN 3855-32-1)[a]

Property (unit)	Value
Boiling point (ºC)	239.2[b]–277[c]
Melting point (ºC)	No data
Density (g/cm^3)	0.83[c]–0.868[b]
Vapor pressure (Pa at 25ºC)	No data
pH (unitless)	No data
Solubility in water (g/100 mL at 25ºC)	No data
Relative vapor density (air = 1)	No data
Molecular weight (g/mol)	201.36

[a]U.S. EPA (2010a).
[b]Physicochemical property predicted by ACD/Labs (RSC, 2010).
[c]Huntsman International (2010).

No reference dose (RfD), reference concentration (RfC), or cancer assessment for pentamethyl dipropylenetriamine is included on the IRIS database (U.S. EPA, 2010b) or on the Drinking Water Standards and Health Advisories List (U.S. EPA, 2009). No RfD or RfC values are reported in the Health Effects Assessment Summary Tables (HEAST) (U.S. EPA, 2003) for pentamethyl dipropylenetriamine. The Chemical Assessments and Related Activities (CARA) list does not include a Health and Environmental Effects Profile (HEEP) for pentamethyl dipropylenetriamine (U.S. EPA, 1994). The toxicity of pentamethyl dipropylenetriamine has not been reviewed by the Agency for Toxic Substances and Disease Registry (ATSDR, 2010) or the World Health Organization (WHO, 2010). The California Environmental Protection Agency

(CalEPA, 2008, 2009) has not derived toxicity values for exposure to pentamethyl dipropylenetriamine. No occupational exposure limits for pentamethyl dipropylenetriamine have been derived by the American Conference of Governmental Industrial Hygienists (ACGIH, 2010), listed by the National Institute of Occupational Safety and Health (NIOSH, 2005), or adopted by the Occupational Safety and Health Administration (OSHA, 2010).

The HEAST (U.S. EPA, 2003) does not report an EPA (1986) cancer weight-of-evidence classification for pentamethyl dipropylenetriamine. The International Agency for Research on Cancer (IARC, 2010) has not reviewed the carcinogenic potential of pentamethyl dipropylenetriamine. Pentamethyl dipropylenetriamine is not included in the *11th Report on Carcinogens* (NTP, 2005). CalEPA (2009) has not prepared a quantitative estimate of carcinogenic potential for pentamethyl dipropylenetriamine.

Literature searches were conducted on sources published from 1900 through February 4, 2011, for studies relevant to the derivation of provisional toxicity values for pentamethyl dipropylenetriamine, CAS No. 3855-32-1. Searches were conducted using EPA's Health and Environmental Research Online (HERO) database of scientific literature. HERO searches the following databases: AGRICOLA; American Chemical Society; BioOne; Cochrane Library; DOE: Energy Information Administration, Information Bridge, and Energy Citations Database; EBSCO: Academic Search Complete; GeoRef Preview; GPO: Government Printing Office; Informaworld; IngentaConnect; J-STAGE: Japan Science & Technology; JSTOR: Mathematics & Statistics and Life Sciences; NSCEP/NEPIS (EPA publications available through the National Service Center for Environmental Publications [NSCEP] and National Environmental Publications Internet Site [NEPIS] database); PubMed: MEDLINE and CANCERLIT databases; SAGE; Science Direct; Scirus; Scitopia; SpringerLink; TOXNET (Toxicology Data Network): ANEUPL, CCRIS, ChemIDplus, CIS, CRISP, DART, EMIC, EPIDEM, ETICBACK, FEDRIP, GENE-TOX, HAPAB, HEEP, HMTC, HSDB, IRIS, ITER, LactMed, Multi-Database Search, NIOSH, NTIS, PESTAB, PPBIB, RISKLINE, TRI; and TSCATS; Virtual Health Library; Web of Science (searches Current Content database among others); World Health Organization; and Worldwide Science. The following databases outside of HERO were searched for risk assessment values: ACGIH, ATSDR, CalEPA, EPA IRIS, EPA HEAST, EPA HEEP, EPA OW, EPA TSCATS/TSCATS2, NIOSH, NTP, OSHA, and RTECS.

REVIEW OF POTENTIALLY RELEVANT DATA (CANCER AND NONCANCER)

The literature search revealed no human or animal studies (i.e., either acute, short term, or chronic) for development of toxicity values for pentamethyl dipropylenetriamine.

DERIVATION OF PROVISIONAL VALUES

Limitations in the available data preclude development of either cancer and noncancer toxicity values for pentamethyl dipropylenetriamine.

CANCER WEIGHT OF EVIDENCE (WOE) DESCRIPTOR

Limitations in the available data preclude development of a WOE descriptor.

MODE-OF-ACTION (MOA) DISCUSSION

Limitations in the available data preclude determination of a MOA discussion.

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