



CHEMICAL UPDATE WORKSHEET

Chemical Name:	t-Amyl methyl ether
CAS #:	994-05-8
Revised By:	RRD Toxicology Unit
Revision Date:	September 24, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	102.18	102.18	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	NA	-80	PC	EXP
Boiling Point (°C)	187	86.30	EPI	EXP
Solubility (ug/L)	2.64E+6	1.0700E+07	PP	EXP
Vapor Pressure (mmHg at 25°C)	75.21	7.52E+01	EPI	EXP
HLC (atm-m³/mol at 25°C)	2.68E-3	1.32E-03	EPI	EXP
Log Kow (log P; octanol-water)	1.73	1.55	PP	EXP
Koc (organic carbon; L/Kg)	28.1	22.66	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.08	6.73E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	8.0E-6	8.0573E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	NA	-7	PC	EXP
Lower Explosivity Level (LEL; unitless)	NA	0.011	PC	EXP
Critical Temperature (K)		536	CRC	EXP
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm ³)		0.766	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	2.61E-05	2.73E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	6.06E-05	6.42E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	3.70E-05	4.33E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	8.45E-05	9.99E-05	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.3E-1	1.3E-1	MDEQ, 2001	
RfD details	<p>Exxon Chemical Americas (1995). Twenty male and twenty female Sprague-Dawley rats aged 6-8 weeks were given TAME by gavage 7 days/wk. for 29 days. Animals received 0, 125, 500, or 1000 mg/kg/day TAME. The critical effect observed was a significant increase in adrenal weights and relative kidney and adrenal weights at 500 mg/kg dose level. The NOAEL for this study is 125 mg/kg/day. UF of 1000 (10 each for inter- and interspecies differences and an</p>	<p>Tier 3 Source: MDEQ: Basis: MDEQ (2001) and Massachusetts (2006) are the same and represent the best available information. Texas RfD is based on an LD50 and ECHA value is not a RfD. MDEQ is selected as the basis because documentation is more thorough. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: RRD 2001 Critical Study: Exxon Chemical Americas, 1995 (unpublished) Method(s): Twenty male and twenty female Sprague-Dawley rats aged 6-8 weeks were given TAME by gavage 7 days/wk. for 29 days. Animals received 0, 125, 500, or 1000 mg/kg/day TAME. Critical effect: increase in adrenal weights and relative kidney and adrenal weights End point or Point of Departure (POD): NOAEL = 125 mg/kg/day Uncertainty Factors: UF = 1000 (10 each for intraspecies variability, interspecies extrapolation and use of a less-than chronic study). Source and date: MDEQ-CCD/RRD, 8/20/2001.</p> <p>Massachusetts DEP, 2006 Drinking Water Regulatory Limit of 0.09 mg/L based on an RfD of 0.125 mg/kg/day; UF = 1000 (10 = subchronic to chronic; 10 each for inter- and intraspecies variation. Based on a 28 day subchronic oral rat study: 125, 500 or 1000 mg/kg/day via gavage for 7 days/week for 28 days. Dose-related</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	additional 10 for a less-than chronic study). MDEQ-RD, 8/20/2001.	<p>statistically significant increases in adrenal and kidney weights were seen at the two higher doses in males. ORS identified a NOAEL of 125 mg/kg/day. Basis same as the DEQ RfD.</p> <p>Texas (TCEQ) – Summary of Updates to the Tables Accompanying the Texas Risk Reduction Program (TRRP) Rule) RfD = 4E-2 mg/kg-day. Based on an oral rat LD50 from the HSDB; NOAEL (?) = 125 mg/kg-day; UF = 3000.</p> <p>ECHA: General population – hazard via oral route. 1 mg/kg bw/day from a repeated dose toxicity study. Reference for the study was not provided and a different risk assessment process from the US process was used. Not pursued.</p> <p>Other Tier 3: No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, Minnesota, New Jersey and New York, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM) and OECD HPV.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	NA	<p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD, no value at this time. Massachusetts DEP: RfD= 0.125 mg/kg/day based on Massachusetts DEP, 2006 Drinking Water Regulatory Limit 0.09 mg/L Texas CEQ: RfD= 4.0E-02 mg/kg/day Justification: NOAEL = 125 mg/kg-day Uncertainty Factors: 10 - Interspecies Extrapolation 10 - Interspecies Extrapolation 10 - Use of Subchronic Study</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		3 - Database Deficiencies Source: A search of the Hazardous Substances Data Bank resulted in little useful data except for a rat LD50 ECHA (REACH): RfD= 1 mg/kg bw/day based on a different risk assessment process.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	6.2E+1	6.2E+1	MDEQ, 2001	
RfC/ITSL details	<p>ITSL based on 13-week inhalation study. In this study the NOEL for female rats was 250 ppm and LOAEL for male rats was 250 ppm. For males there was an increase in the absolute liver weight and liver to body weight and liver to brain weight ratios. For male mice the NOEL was 250 ppm, while the LOAEL for female mice was 250 ppm. For</p>	<p>Tier 3 Source: MDEQ: Basis: MDEQ RfC is the best available endpoint ; only REACH-ECHA had a value but it was one derived by a different risk assessment process than conducted in the US. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: 2001 ITSL = 6.2E+1 $\mu\text{g}/\text{m}^3$ with 24 hour averaging time Critical Study: API, 1997 Method(s): Male and female Fischer-344 rats and CD-1 mice were exposed to 0, 250, 1500, or 3500 ppm of tertiary amyl methyl ether for 6 hrs. /day, 5 days/wk. for 13 weeks. There were 51 rats/sex/group in the control and high-exposure groups and 41 rats/sex/group in the low- and mid-exposure groups. For mice there were 46 animals in the control and high-exposure groups and 36 animals in the low-and mid-exposure groups. Critical effects: increase in the absolute liver weight and liver to body weight and</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	<p>females, there was an increase in labeling index of hepatocytes. The ITSL was based on the LOAEL for male rats and female mice with a 3000 uncertainty factor. AQD calculation date: 4/26/2001.</p>	<p>liver to brain weight ratios for male rats and increase in labeling index of hepatocytes for female mice End point or Point of Departure (POD): LOAEL for male rats and female mice = 250 ppm; The NOEL for female rats was 250 ppm and LOAEL for male rats was 250 ppm. Averaging time = 24 hours. Uncertainty Factors: UF = 3000 (10 each for intraspecies variability, interspecies extrapolation, and LOAEL to NOAEL extrapolation, and 3 for use of a less-than chronic study). Source and date: MDEQ-AQD, 4/26/2001.</p> <p>ECHA (REACH): The information provided appears to be based on the same study as the MDEQ value; however, the reference is not provided and a RfC is not reported as a different risk assessment process is utilized. A NOAEC of 250 ppm is reported as well as a DNEL (Derived No Effect Level) of 26.5 mg/m³. The DNEL is for the general population hazard via inhalation route. The assessment process is not directly comparable to the risk assessment process in the US and thus, was not pursued further.</p> <p>Other Tier 3: No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, Massachusetts, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
Developmental or Reproductive Effector? (Y/N)	No	No, the RfD is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard (SDWS) (ug/L)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (ug/L)	--	NO	SDWA, 1976 and USEPA SMCL List	
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
Is there an aesthetic value for drinking water? (Y/N)	YES	YES	NA	
Aesthetic value (ug/L)	194	194	MDEQ-RRD, 2015	
Aesthetic Value details	Aesthetic value was not recorded in MDEQ-CCD.	Aesthetic criterion based on odor described as sweet, rubbery, fruity, ether-like, and paint-like. DW date: 10/30/2001 Note: Aesthetic value was not recorded in MDEQ-CCD.		
Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	NA	NA	NA	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Others				

(C) Chemical-specific Absorption Factors

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABS _{gi})	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS _{gi} details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (AE _d)	---	0.1	MDEQ, 2015/USEPA RAGS-E, 2004	
AE _d details		RAGS E (USEPA, 2004): There is no default value assigned for inorganics because the speciation of the compound is critical to the dermal absorption and there are too little data to extrapolate a reasonable default value.		
Ingestion Absorption Efficiency (AE _i)		1.0	MDEQ, 2015	
AE _i Details				
Relative Source Contribution for Water (RSC _w)		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC _s)		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC _A)		1.0	MDEQ, 2015	
Others				

(D) Rule 57 Water Quality Values and GSI Criteria

Current GSI value (µg/L)	NA
Updated GSI value (µg/L)	NA
Rule 57 Drinking Water Value (µg/L)	NA

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)		
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)		
Wildlife Value (WV)		
Human Cancer Values for Drinking Water Source (HCV-drink)		
Human Cancer values for non-drinking water source (HCV-Non-drink)		
Final Chronic Value (FCV)		
Aquatic maximum value (AMV)		
Final Acute Value (FAV)		

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)



(E) Target Detection Limits (TDL)

	Value	Source
Target Detection Limit – Soil ($\mu\text{g}/\text{kg}$)	250	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	5	MDEQ, 2015
Target Detection Limit – Air (ppbv)	1.50E+01	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	4.90E+02	MDEQ, 2015

CHEMICAL UPDATE WORKSHEET ABBREVIATIONS:

CAS # - Chemical Abstract Service Number.

Section (A) Chemical-Physical Properties**Reference Source(s):**

CRC	Chemical Rubber Company Handbook of Chemistry and Physics, 95th edition, 2014-2015
EMSOFT	USEPA Exposure Model for Soil-Organic Fate and Transport (EMSOFT) (EPA, 2002)
EPA2001	USEPA (2001) Fact Sheet, Correcting the Henry's Law Constant for Soil Temperature. Office of Solid Waste and Emergency Response, Washington, D.C.
EPA4	USEPA (2004) User's Guide for Evaluating Subsurface Vapor Intrusion into Buildings. February 22, 2004.
EPI	USEPA's Estimation Programs Interface SUITE 4.1, Copyright 2000-2012
HSDB	Hazardous Substances Data Bank
MDEQ	Michigan Department of Environmental Quality
NPG	National Institute for Occupational Safety and Health Pocket Guide to Chemical Hazards
PC	National Center for Biotechnology Information's PubChem database
PP	Syracuse Research Corporation's PhysProp database
SCDM	USEPA's Superfund Chemical Data Matrix
SSG	USEPA's Soil Screening Guidance: Technical Background Document, Second Edition, 1996
USEPA/EPA	United States environmental protection agency's Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment). July, 2004.

W9 USEPA's User Guide for Water9 Software, Version 2.0.0, 2001

Basis/Comments:

EST	estimated
EXP	experimental
EXT	extrapolated
NA	not available or not applicable
NR	not relevant

Section (B) Toxicity Values/Benchmarks**Sources/References:**

ATSDR	Agency for Toxic Substances and Disease Registry
CALEPA	California Environmental Protection Agency
CAL DTSC	California Department of Toxic Substances Control
CAL OEHHA	CAEPA Office of Environmental Health Hazard Assessment
CCD	MDEQ Chemical Criteria Database
ECHA	European Chemicals Agency (REACH)
OECD HPV	Organization for Economic Cooperation and Development HPV Database
HEAST	USEPA's Health Effects Assessment Summary Tables
IRIS	USEPA's Integrated Risk Information System
MADEP	Massachusetts Department of Environmental Protection
MDEQ/DEQ	Michigan Department of Environmental Quality
DEQ-CCD/AQD	MDEQ Air Quality Division
DEQ-CCD/RRD	MDEQ Remediation and Redevelopment Division
DEQ-CCD/WRD	MDEQ Water Resources Division
MNDOH	Minnesota Department of Health

NJDEP	New Jersey Department of Environmental Protection
NYDEC	New York State Department of Environmental Conservation
OPP/OPPT	USEPA's Office of Pesticide Programs
PPRTV	USEPA's Provisional Peer Reviewed Toxicity Values
RIVM	The Netherlands National Institute of Public Health and the Environment
TCEQ	Texas Commission on Environmental Quality
USEPA	United States Environmental Protection Agency
USEPA OSWER	USEPA Office of Solid Waste and Emergency Response
USEPA MCL	USEPA Maximum Contaminant Level
WHO	World Health Organization
WHO IPCS	International Programme on Chemical Safety (IPCS/INCHEM)
WHO IARC	International Agency for Research on Cancers
NA	Not Available.
NR	Not Relevant.

Toxicity terms:

BMC	Benchmark concentration
BMCL	Lower bound confidence limit on the BMC
BMD	benchmark dose
BMDL	Lower bound confidence limit on the BMD
CSF	Cancer slope Factor
CNS	Central nervous system
IURF or IUR	Inhalation unit risk factor
LOAEL	Lowest observed adverse effect level
LOEL	Lowest observed effect level
MRL	Minimal risk level (ATSDR)
NOAEL	No observed adverse effect level
NOEL	No observed effect level

RfC	Reference concentration
RfD	Reference dose
p-RfD	Provisional RfD
aRfD	Acute RfD
UF	Uncertainty factor
WOE	Weight of evidence

Section (C) Chemical-specific Absorption Factors

MDEQ	Michigan Department of Environmental Quality
USEPA RAGS-E	United States Environmental Protection Agency's Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment). July, 2004.

Section (D) Rule 57 Water Quality Values and GSI Criteria

GSI	Groundwater-surface water interface
NA	A value is not available or not applicable.
ID	Insufficient data to derive value
NLS	No literature search has been conducted