



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>Aniline</b>
<b>CAS #:</b>	<b>62-53-3</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	September 24, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	93.13	93.13	EPI	EXP
<b>Physical State at ambient temp</b>	Liquid	Liquid	MDEQ	
<b>Melting Point (°C)</b>	257	-6.02	EPI	EXP
<b>Boiling Point (°C)</b>	184.1	184.17	EPI	EXP
<b>Solubility (ug/L)</b>	3.60E+7	3.6000E+07	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	0.6688	6.67E-01	EPI	EXP
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	2.30E-6	2.02E-06	EPI	EXP
<b>Log Kow (log P; octanol-water)</b>	0.978	0.90	EPI	EXP
<b>Koc (organic carbon; L/Kg)</b>	9.15	70.23	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.07	8.30E-02	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.3E-6	1.0125E-05	W9	EST
<b>Soil Water Partition Coefficient (Kd; inorganics)</b>	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	158 F	70	CRC	EXP
Lower Explosivity Level (LEL; unit less)	0.013	0.013	CRC	EXP
Critical Temperature (K)		704	CRC	EXP
Enthalpy of Vaporization (cal/mol)		1.01E+04	CRC	EXP
Density (g/mL, g/cm <sup>3</sup> )		1.0217	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	7.57E-06	7.08E-06	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	7.58E-06	7.08E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	9.06E-06	8.96E-06	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	9.06E-06	8.96E-06	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	NA	7.0E-3	PPRTV, 2007	
RfD details		<p><b>Tier 2 Source:</b>  <b>PPRTV:</b>  <b>Basis:</b> PPRTV is a Tier 2 source. No Tier 1 value.  <b>PPRTV (5/23/2007)</b> p-RfD = 7.0E-3.  <b>Critical Study:</b> CIIT (Chemical Industry Institute of Toxicology). 1982. 104-Week chronic toxicity study in rats. Aniline hydrochloride. Prepared for CIIT, Research Triangle Park, NC by Hazleton Laboratories America, Inc., Vienna, VA. Submitted to U.S. EPA under TSCA Section 8D. EPA Doc. No. 878212078. Fiche No. OTS 205944. TSCATS 16580. (Unpublished)  <b>Method(s):</b> CD-1 rats (130/sex) were fed diets containing aniline hydrochloride at target doses 0, 10, 30 or 100 mg/kg-day for 104 weeks.  <b>Critical effect:</b> Hematological and splenic effects in rats  <b>End point or Point of Departure (POD):</b> LOAEL = 10 mg/kg-day of aniline hydrochloride. The 10 mg/kg-day dose of aniline hydrochloride is converted into an equivalent dose of aniline (7 mg/kg-day); The p-RfD for aniline hydrochloride would be 1E-2 mg/kg-day  <b>Uncertainty Factors:</b> UF = 1,000 (10 to account for interspecies extrapolation, 10 for human variability and 3 to account for lack of a reproductive and multigenerational developmental study).  <b>Source and date:</b> PPRTV; 5/23/2007</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> Per IRIS (9/07/1988), no value at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD/WRD (8/26/1998), RfD = 0.006888 mg/kg-day (6.9E-3).  <b>Critical Studies:</b> CIIT (Chemical Industry Institute of Toxicology). 1982. 104-Week chronic toxicity study in rats. Aniline hydrochloride. Prepared for CIIT, Research</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		Triangle Park, NC by Hazleton Laboratories America, Inc., Vienna, VA. Submitted to U.S. EPA under TSCA Section 8D. EPA Doc. No. 878212078. Fiche No. OTS 205944. TSCATS 16580. (Unpublished) <b>Method(s):</b> CD-1 rats (130/sex) were fed diets containing aniline hydrochloride at target doses 0, 10, 30 or 100 mg/kg-day for 104 weeks. <b>Critical effect:</b> Hematological and splenic effects in rats <b>End point or Point of Departure (POD):</b> LOAEL = 9.572 mg/kg-day <b>Uncertainty Factors:</b> UF = 1,000 (10 each for intra-species variability and interspecies extrapolation and 3 for LOAEL to NOAEL) <b>Source and date:</b> MDEQ-CCD/WRD, 9/18/1998		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	1.6E-2	5.7E-3	IRIS, 1994	
<b>CSF details</b>	Fibrosarcoma, stromal sarcoma, capsular sarcoma, and hemangiosarcoma of the spleen in male F344 rats following aniline. HCL exposure via the diet for 104 weeks (CIIT, 1982). The potency calculated for aniline HCl was modified in order to derive potency for aniline. Revised species scaling factor of	<b>Tier 1 Source:</b> <b>IRIS:</b> <b>Basis:</b> IRIS is a Tier 1 source and the only available value. <b>IRIS (02/01/1994) CSF = 5.7E-3 (mg/kg-day)<sup>-1</sup>.</b> <b>Critical Study:</b> CIIT (Chemical Industry Institute of Toxicology). 1982. 104-Week chronic toxicity study in rats: Aniline hydrochloride. Final report. <b>Method(s):</b> Male and female CD-F rats (130/sex/dose) were exposed to aniline hydrochloride in diet at levels of 0, 200, 600 and 2000 ppm for 2 years. 1) <i>Dose response data: Tumor Type</i> - combined fibrosarcoma, stromal sarcoma, capsular sarcoma and hemangiosarcoma in the spleen; <i>Test Species</i> - rats; <i>Route</i> - diet 2) <i>Extrapolation method:</i> Linearized multistage procedure, extra risk <b>Carcinogen Weight-of-Evidence (WOE) Class:</b> B2; probable human carcinogen <b>IRIS WOE Basis:</b> Induction of tumors of the spleen and the body cavity in two strains of rat, and some supporting genetic toxicological evidence <b>Source and Date:</b> IRIS; Last revision date - 02/01/94. EPA conducted a literature review in September, 2002 and did not identify any critical new studies <b>Tier 2 Sources:</b> <b>PPRTV:</b> PPRTV (5/23/2007) supports the IRIS CSF.		Complete

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	(BWh/BWa) to the 0.25 power used for q* calculation.	<b>MRL:</b> NA; MRLs are for non-cancer effects only. <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no value at this time, the IRIS value when applied the revised species scaling factor yields a slope factor of 1.6E-2 per mg/kg/day.		
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (<math>\mu\text{g}/\text{m}^3</math>)</b>	1.0E+0	1.0E+0	IRIS, 1993	
<b>RfC/ITSL details</b>	Based on EPA's IRIS. Oberst et al 1956 NOAEL of 3.4 mg/m <sup>3</sup> and the duPont deNemours 1982 (unpublished) LOAEL of 11.6 mg/m <sup>3</sup> . CCD/AQD date: 9/20/1990  4/17/2012 Update Second ITSL based on TLV of 7.6 mg/m <sup>3</sup> (methemoglobinemia). . ;	<b>Tier 1 Source:</b> <b>IRIS:</b> <b>Basis:</b> IRIS is a Tier 1 source and the only available value. <b>IRIS RfC</b> = 1.0E-3 mg/m <sup>3</sup> . <b>Critical Studies:</b> 1) Oberst F.W., E. Hackley, C. Comstock. 1956. Chronic toxicity of aniline vapor (5 ppm) by inhalation. Arch. Ind. Health. 13: 379-384. 2) duPont deNemours and Company, Inc. 1982. Subacute inhalation toxicity study of aniline in rats. OTS No. 878220240. Fiche No. 0215025. (unpublished) <b>Method(s):</b> 1) Whole body exposure of 9 male Wistar rats and 2 dogs for 26 weeks, and 20 female albino mice and 10 guinea pigs for 20 weeks, to 5 ppm (19 mg/m <sup>3</sup> ) of aniline vapor for 6 hours/day, 5 days/week. 2) Male Crl:CD rats (16/group) were exposed (head-only) to 0, 17, 45, or 87 ppm aniline vapors, 6 hours/day, 5 days/week, for 2 weeks <b>Critical effect:</b> 1) lack of toxicity (Oberst, 1956) and 2) mild spleen toxicity (DuPont, 1982) <b>End point or Point of Departure (POD):</b> 1) NOAEL = 19 mg/m <sup>3</sup> ; NOAEL <sub>ADJ</sub> = 3.4 mg/m <sup>3</sup> ; NOAEL <sub>HEC</sub> = 3.4 mg/m <sup>3</sup> 2) LOAEL = 64.7 mg/m <sup>3</sup> ; LOAEL <sub>ADJ</sub> = 11.6 mg/m <sup>3</sup> ; LOAEL <sub>HEC</sub> = 11.6 mg/m <sup>3</sup> <b>Uncertainty Factors:</b> UF = 3,000; (10 each for intra-species variability, interspecies extrapolation and use of a subchronic study and 3 for lack of		Complete

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		reproductive studies) <b>Source and date:</b> IRIS, Last revision date - 12/01/1993  <b>Tier 2 Sources:</b> <b>PPRTV:</b> PPRTV (5/23/2007) supports the IRIS RfC. <b>MRL:</b> No MRL record available at this time.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD (4/17/2012), AQD adopted IRIS RfC.		
<b>Inhalation Unit Risk Factor (IURF) ((<math>\mu\text{g}/\text{m}^3</math>)<sup>-1</sup>)</b>	--	1.6E-6	MDEQ, 2012	
<b>IURF details</b>	EPA IRIS 6/3/87 identifies oral potency of 5.7 E-3 (mg/kg)-1.	<b>Tier 3 Source:</b> <b>MDEQ:</b> <b>Basis:</b> MDEQ and CA values are the same/based on the same data. Better documentation for the MDEQ value. See details below.  <b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> Per IRIS (2/01/1994), no value at this time. <b>PPRTV:</b> Per PPRTV (5/23/2007), no PPRTV value. <b>MRL:</b> NA; MRLs are for non-cancer effects only.  <b>Tier 3 Sources:</b> <b>MDEQ:</b> Per CCD/AQD, IURF = 1.6E-6 ( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup> <b>Basis:</b> IURF is based on the conversion of the IRIS oral slope factor to IURF. See Updated Value CSF Details. <b>Source and date:</b> MDEQ-AQD, 4/17/2012.  <b>California DTSC:</b> IURF= 0.0000016 ( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup> based on male rat spleen tumor data (CIIT, 1982). The CIIT study is an oral study and the slope factor of 5.7E-3 (mg/kg-day) <sup>-1</sup> was converted to an inhalation dose (assumes 70 kg body weight and 20 m <sup>3</sup> /day inhalation rate).	Complete	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<b>Other Tier 3:</b> No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of Massachusetts, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.		
<b>Mutagenic Mode of Action (MMOA)? (Y/N)</b>	--	NO	USEPA, 2015	
<b>MMOA Details</b>	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
<b>Developmental or Reproductive Effector? (Y/N)</b>	No	No, the RfD or RfC/ITSL is not based on a reproductive-developmental effect.	MDEQ, 2015	
<b>Developmental or Reproductive Toxicity Details</b>	NA	NA		
<b>State Drinking Water Standard (SDWS) (ug/L)</b>	NO	NO		
<b>SDWS details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399; US EPA MCL and SMCL Lists		
<b>Secondary Maximum Contaminant Level (SMCL) (ug/L)</b>	--	NO	SDWA, 1976 and USEPA SMCL List	
<b>SMCL details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
<b>Aesthetic value (ug/L)</b>	--	NA	NA	
<b>Aesthetic value details</b>	NA	NA		
<b>Is there an aesthetic value for drinking water? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Aesthetic Value details</b>	NA	NA		

	<b>Part 201 Value</b>	<b>Updated Value</b>	<b>Source/Reference/ Date</b>	<b>Comments/Notes /Issues</b>
<b>Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Phytotoxicity details</b>	NA	NA	NA	
<b>Others</b>				

**(C) Chemical-specific Absorption Factors**

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABS <sub>gi</sub> )	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS <sub>gi</sub> details		MDEQ, 2015/USEPA RAGS-E, 2004		
Skin absorption efficiency value (AE <sub>d</sub> )	---	0.1	MDEQ, 2015	
AE <sub>d</sub> details				
Ingestion Absorption Efficiency (AE <sub>i</sub> )		1.0	MDEQ, 2015	
AE <sub>i</sub> Details				
Relative Source Contribution for Water (RSC <sub>w</sub> )		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC <sub>s</sub> )		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC <sub>A</sub> )		1.0	MDEQ, 2015	
Others				

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

<b>Current GSI value (µg/L)</b>	4
<b>Updated GSI value (µg/L)</b>	4
<b>Rule 57 Drinking Water Value (µg/L)</b>	21

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	190	9/1998
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	13,000	9/1998
<b>Wildlife Value (WV)</b>	NA	NA
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	21	9/1998
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	1,500	9/1998
<b>Final Chronic Value (FCV)</b>	4	7/1999
<b>Aquatic maximum value (AMV)</b>	18	7/1999
<b>Final Acute Value (FAV)</b>	36	7/1999

Sources:

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

**(E) Target Detection Limits (TDL)**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	330	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	4	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	NA	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	NA	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 OEHHHA	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