n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

Prepared by:

ToxServices LLC

October 16, 2014

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TABLE OF CONTENTS

TABLE OF FIGURES

TABLE OF TABLES

GreenScreen® Executive Summary for n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)

n-Ethyl-o (or p)-toluenesulfonamide is a chemical that has unknown functions.

n-Ethyl-o (or p)-toluenesulfonamide was assigned a GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") as it has Moderate Group I Human Health hazard (reproductive toxicity (R) and developmental toxicity (D)), High Group II Human Health hazard (single dose neurotoxicity (Ns)), High Ecotoxicity (chronic aquatic toxicity (CA)), and High persistence (P). This corresponds to GreenScreen® benchmark classifications 2c ("High P + Moderate T (Ecotoxicity or Group I, II, or II* Human)") and 2e ("Moderate T (Group I Human)") in CPA 2011. Data gaps (DG) exist for endocrine activity (E) and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Conduct a Data Gap Analysis to assign a final Benchmark score), n-ethyl-o (or p)-toluenesulfonamide meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if n-ethyl-o (or p)-toluenesulfonamide were assigned a score of High for the data gap endocrine activity (E), it would be categorized as a Benchmark 1 Chemical.

GreenScreen® Benchmark Score for Relevant Route of Exposure:
As a standard approach for GreenScreen® evaluations, all exposure routes (oral, dermal, and inhalation) were evaluated together, so the GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") is applicable for all routes of exposure.

GreenScreen® Hazard Ratings for n-Ethyl-o (or p)-toluenesulfonamide

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	**L**	**M**	**M**	DG	**L**	**L**	**L**	**H**	**L**	**L**	DG	**L**	**M**	**M**	*H*	*H*	**vL**	*L*	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Assessment for n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)

Method Version: GreenScreen® Version 1.2[1]
Assessment Type[2]: Certified

Chemical Name: n-Ethyl-o (or p)-toluenesulfonamide

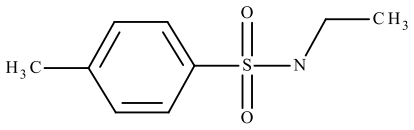
CAS Number: 8047-99-2

GreenScreen® Assessment Prepared By:
Name: Zach Guerrette, Ph.D.
Sara Ciotti, Ph.D.
Title: Toxicologists
Organization: ToxServices LLC
Date: October 15, 2014
Assessor Type: Licensed GreenScreen® Profiler

Quality Control Performed By:
Name: Bingxuan Wang, Ph.D.
Title: Toxicologist
Organization: ToxServices LLC
Date: October 16, 2014

Confirm application of the *de minimus* rule[3]: N/A

Chemical Structure(s):



(CAS #8047-99-2)

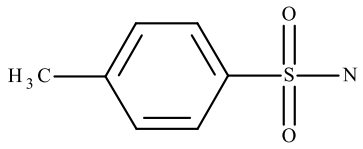
Also called:
Toluene ethylsulfonamide; EINECS 232-465-2; N-Ethyl-2(or 4)-methylbenzenesulfonamide; N-Ethyl-o(or p)-toluenesulfonamide; Benzenesulfonamide, N-ethyl-2(or 4)-methyl-; N-Ethyl-o(or p)-toluenesulphonamide; N-Ethyltoluenesulfonamide (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
Limited data were identified for n-ethyl-o (or p)-toluenesulfonamide and the individual components n-ethyl-p-toluenesulfonamide and n-ethyl-o-toluenesulfonamide. ToxServices identified potential chemical surrogates using the structural similarity search function of ChemIDplus and the U.S. EPA's Analog Identification Methodology (AIM) software. Using this approach, ToxServices identified p-toluenesulfonamide (CAS #70-55-3) as a suitable surrogate based on the similar p-toluenesulfonamide core of n-ethyl-o (or p)-toluenesulfonamide, similar molecular weight (171.2191 g/mol for p-toluenesulfonamide and 199.2727 g/mol for n-ethyl-o (or p)-toluenesulfonamide), and availability of data. Data for p-toluenesulfonamide were used to address the data gaps for n-ethyl-o (or p)-toluenesulfonamide.

[1] Use GreenScreen® Assessment Procedure (Guidance) V1.2

[2] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent) or "CERTIFIED WITH VERIFICATION" (Certified or Authorized assessment that has passed GreenScreen® Verification Program)

[3] Every chemical in a material or formulation should be assessed if it is:
1. intentionally added and/or
2. present at greater than or equal to 100 ppm



(CAS #70-55-3)

Identify Applications/Functional Uses:
No uses were identified for n-ethyl-o (or p)-toluenesulfonamide.

GreenScreen® Summary Rating for n-Ethyl-o (or p)-toluenesulfonamide[4]: n-Ethyl-o (or p)-toluenesulfonamide was assigned a GreenScreen® Benchmark Score of 2 ("Use but Search for Safer Substitutes") as it has Moderate Group I Human Health hazard (reproductive toxicity (R) and developmental toxicity (D)), High Group II Human Health hazard (single dose neurotoxicity (Ns)), High Ecotoxicity (chronic aquatic toxicity (CA)), and High persistence (P). This corresponds to GreenScreen® benchmark classifications 2c ("High P + Moderate T (Ecotoxicity or Group I, II, or II* Human)") and 2e ("Moderate T (Group I Human)") in CPA 2011, 2012a. Data gaps (DG) exist for endocrine activity (E) and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Conduct a Data Gap Analysis to assign a final Benchmark score), n-ethyl-o (or p)-toluenesulfonamide meets requirements for a GreenScreen® Benchmark Score of 2 despite the hazard data gaps. In a worst-case scenario, if n-ethyl-o (or p)-toluenesulfonamide were assigned a score of High for the data gap endocrine activity (E), it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Ratings for n-Ethyl-o (or p)-toluenesulfonamide

Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	L	M	M	DG	L	L	L	H	L	L	DG	L	M	M	H	*H*	vL	*M*	L

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated (modeled) values, authoritative B lists, screening lists, weak analogues and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e. vH, H, M, and L) instead of three (i.e. H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

Transformation Products and Ratings:
Identify feasible and relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) **and/or moieties of concern**[5]

No transformation products were identified in the available literature for n-ethyl-o (or p)-toluenesulfonamide. Modeling with OECD QSAR Toolbox (OECD 2013) did not identify any

[4] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.
[5] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

hydrolysis products for this chemical. Based on the lack of feasible transformation products, the Benchmark Score for n-ethyl-o (or p)-toluenesulfonamide is not adjusted by transformation products.

Introduction

n-Ethyl-o (or p)-toluenesulfonamide is a mixture of n-ethyl-o-toluenesulfonamide (CAS #1077-56-1) and n-ethyl-p-toluenesulfonamide (CAS #80-39-7). No information on the uses or production of n-ethyl-o (or p)-toluenesulfonamide was identified.

ToxServices assessed n-ethyl-o (or p)-toluenesulfonamide against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.69 (GreenScreen® Hazard Assessment) (ToxServices 2013).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2014) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. It checks all of the lists in the List Translator with the exception of the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b) and these should be checked separately in conjunction with running the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for n-ethyl-o (or p)-toluenesulfonamide can be found in Appendix C and a summary of the results can be found below:

- n-Ethyl-o (or p)-toluenesulfonamide is not listed in the Pharos database.
- n-Ethyl-o (or p)-toluenesulfonamide is not listed in the U.S. DOT (2008a,b) lists.

Physicochemical Properties of n-Ethyl-o (or p)-toluenesulfonamide

n-Ethyl-o (or p)-toluenesulfonamide is a clear oily liquid under standard temperature and pressure. It has a vapor pressure of 10 mm Hg, indicating that it will exist mostly in the vapor phase. It is practically insoluble in water.

Table 1: Physical and Chemical Properties of n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)]

Property	Value	Reference
Molecular formula	C9-H13-N-O2-S	ChemIDplus 2014
SMILES Notation	c1(S(NCC)(=O)=O)ccc(C)cc1	ChemIDplus 2014
Molecular weight	199.2727 g/mol	ChemIDplus 2014
Physical state	Liquid	Unitex 2009
Appearance	Clear, oily	Unitex 2009
Melting point	Not identified	
Vapor pressure	10 mm Hg at 196°C	Unitex 2009
Water solubility	Practically insoluble	Unitex 2009
Dissociation constant	Not identified	
Density/specific gravity	Specific gravity = 1.19	Unitex 2009
Partition coefficient	Not identified	

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): *L*
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for carcinogenicity based on the lack of structural alerts for genotoxic and non-genotoxic carcinogenicity. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when negative data, no structural alerts, and no GHS classification are available (CPA 2012a). The confidence in the score is adjusted as it is based on modeling.

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint. ToxServices performed modeling to predict the carcinogenic potential of n-ethyl-o (or p)-toluenesulfonamide. ToxServices also attempted to use the OncoLogic program, but this chemical does not belong to any of the chemical categories in the program.
  - ToxTree 2013
    - No structural alerts for genotoxic or non-genotoxic carcinogenicity were identified for n-ethyl-o (or p)-toluenesulfonamide (see Appendix D).
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - No data were identified for this endpoint.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): L
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for mutagenicity/genotoxicity based on negative results for mutagenicity and clastogenicity for n-ethyl-o (or p)-toluenesulfonamide and the surrogate p-toluenesulfonamide. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when negative data for mutagenicity and clastogenicity, no structural alerts, and no GHS classification are available (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - Zeiger et al. 1992
    - *In vitro*: Negative results for mutagenicity were obtained in an Ames test. *Salmonella typhimurium* tester strains TA 97, TA 98, TA 100, and TA 1535 were exposed to n-ethyl-o (or p)-toluenesulfonamide (purity not specified) at 33-2,000 µg/plate with and without metabolic activation. No increase in the mutation frequency was observed with treatment in the presence or absence of metabolic activation.
  - U.S. EPA 2006
    - *In vivo*: Negative results for clastogenicity were obtained in a GLP-compliant micronucleus test conducted according to OECD 474. Wistar rats (5/sex/dose group) were administered single oral doses of n-ethyl-o (or p)-toluenesulfonamide (purity not specified) at 0, 100, 200, or 400 mg/kg. The animals were sacrificed 24 or 48 hours after dosing and bone marrow samples were isolated for assessment of

micronuclei. No increase in the incidence of micronuclei was observed with treatment.

- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - *In vitro*: Mixed results for mutagenicity were obtained in a GLP-compliant, mammalian cell gene mutation test conducted according to OECD 476. Mouse lymphoma L5178Y cells were exposed to p-toluenesulfonamide (99.9% purity) at 125-5,000 µg/mL with metabolic activation and 31.3-5,000 µg/mL without metabolic activation. No increase in the mutation frequency was observed with treatment in the absence of metabolic activation but an increase in the mutation frequency was observed in the highest dose tested which was also cytotoxic.
      - Although an increase in the mutation frequency was observed in this test with metabolic activation, the increase only occurred at a cytotoxic dose. Therefore, ToxServices discounted the positive result observed in this test.
    - *In vitro*: Negative results for mutagenicity were obtained in a non-GLP-compliant Ames test conducted according to OECD 471. *S. typhimurium* tester strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538 and *Saccharomyces cerevisiae* (strain not specified) were exposed to p-toluenesulfonamide (purity not specified) at 1-1,000 µg/plate with and without metabolic activation. No increase in the mutation frequency was observed with treatment in the presence or absence of metabolic activation.
    - *In vivo*: Negative results for clastogenicity were obtained in a GLP-compliant mouse micronucleus test conducted according to OECD 474. Crl:CD-1 (CR)BR mice (6-12/sex/dose group) were administered single oral doses of p-toluenesulfonamide (99.3% purity) at 0, 187.5, 375, 750, or 1,500 mg/kg. After 48 hours, the animals were sacrificed and bone marrow tissues were isolated for assessment of micronuclei. No increase in the incidence of micronuclei was observed with treatment.

Reproductive Toxicity (R) Score (H, M, or L): M

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Moderate for reproductive toxicity based on difficult delivery in one rat reproductive study performed with the surrogate p-toluenesulfonamide. GreenScreen® criteria classify chemicals as a Moderate hazard for reproductive toxicity when limited or marginal evidence of reproductive toxicity is observed in animals (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - A GLP-compliant two-generation reproductive toxicity study conducted according to OECD 416 was performed with Wistar rats (24/sex/dose group) provided diets containing p-toluenesulfonamide (99.9% purity) at 0, 1,000, 3,000, or 10,000 ppm (equivalent to 0, 52-78, 165-237, and 566-832 mg/kg/day for males and 0, 75-161, 232-499, and 733-1,631 mg/kg/day for females, respectively). The original parental animals (F0 generation) were treated for 10 weeks prior to mating until the end of the study, the F1 animals were exposed in utero through nursing, directly following

weaning and for 10 weeks prior to mating until the end of the study, and the F2 animals were exposed in utero and throughout the lactation period. The animals were evaluated for clinical signs of toxicity, body weight, food and water consumption, sperm parameters, estrous cyclicity, reproductive indices, offspring viability indices, gross pathology, and histopathology. No treatment-related effects were observed on clinical signs of toxicity, estrous cyclicity, sperm parameters, reproductive performance, gross pathology, or histopathology of the parental animals. Decreased body weight and body weight gain were consistently observed in the mid and high dose groups for males and females in the F0 and F1 generations. No treatment-related effects were observed on offspring viability, clinical signs of toxicity, sexual maturation, gross pathology, or histopathology. Decreased body weights were observed for male and female F1 pups in the high dose group and male and female F2 pups in the high dose group. F1 male pups exhibited a delay in balanoperputial separation (external sign of puberty in male rat) (108% of control) and F1 female pups exhibited a delay in vaginal opening (114% of control). The study authors identified a developmental LOAEL of 10,000 ppm (566-832 mg/kg/day for males and 733-1,631 mg/kg/day for females) based on decreased pup weight and delayed sexual maturation in the F1 pups and a reproductive NOAEL of 10,000 ppm (566-832 mg/kg/day for males and 733-1,631 mg/kg/day for females) based on the lack of effects to reproduction observed in the study.

- A GLP-compliant combined repeated dose toxicity study with reproduction developmental toxicity screening test conducted according to OECD 422 was performed with Sprague-Dawley rats (13/sex/dose group) administered oral doses of p-toluenesulfonamide (purity not specified) at 0, 120, 300, or 750 mg/kg/day. The males were dosed for 42 days and the females were dosed for 14 days prior to mating to postnatal day 3. The parental animals were evaluated for clinical signs of toxicity, body weight, estrous cyclicity, and reproductive performance. The offspring were evaluated for viability, clinical signs of toxicity, body weight, gross pathology, and histopathology. No treatment-related effects were observed on mating performance or fertility. In the high dose group, 2/10 females had difficult deliveries and all of their offspring died by postnatal day 3. The duration of gestation, numbers of corpora lutea, implantations and resorptions, litter size, and sex distribution were not affected by treatment. No teratogenic effects were observed with treatment. The survival rate and body weights of offspring in the high dose group were significantly decreased relative to control values. The study authors identified reproductive and developmental LOAELs of 750 mg/kg/day based on the decrease survival and body weight of the offspring in the high dose group. ToxServices assigned the LOAEL at 750 mg/kg/day for reproductive toxicity based on difficult deliveries.

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): M
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Moderate for developmental toxicity based on decreased pup weight, decreased survival, delayed sexual maturation, and/or increased incidence of skeletal anomalies. GreenScreen® criteria classify chemicals as a Moderate hazard for developmental toxicity when limited or marginal evidence of developmental toxicity is observed in animals (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.

- *Screening:* Not listed on any screening lists for this endpoint.

- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - A GLP-compliant prenatal toxicity study conducted in a manner similar to OECD 414 was performed with pregnant female New Zealand White rabbits (27-30/dose group) provided p-toluenesulfonamide (99.9% purity) at 0, 1,000, 3,000, or 11,000 ppm (equivalent to 0, 41, 113, and 367 mg/kg/day, respectively) on gestational days (GD) 7-29. The animals were sacrificed on GD 30. Maternal examinations included clinical signs of toxicity, body weight, food and water consumption, and ovarian and uterine content. Fetal examinations consisted of evaluating the incidence of external, visceral, head, and skeletal malformations. Females in the high dose group exhibited decreased body weight, body weight gain, and food consumption, with the highest magnitude of effect being observed in the first days of treatment (GD 7-10). Females in the mid dose group also exhibited decrease decreased body weight, body weight gain, and food consumption but these effects were of a lesser magnitude and duration than those observed in the high dose group. No treatment-related effects were observed on pre- and post-implantation loss, litter size, or sex ratio. The total number of malformations observed in fetuses (number of litters) was 3 (3), 0 (0), 4 (3), and 11 (8) for the control, low, mid, and high dose groups, respectively. The treatment-related malformations were vertebral anomalies with or without associated rib anomalies. The high dose group fetuses exhibited an increased incidence of this anomaly relative to controls. This finding may also have been related to maternal stress since the incidences of these anomalies coincided with on-site construction that may have affected the females and no skeletal malformations were observed in the range-finding study that tested doses up to 20,000 ppm. The study authors identified a LOAEL of 11,000 ppm (equivalent to 367 mg/kg/day) based on the increased incidence of vertebral anomalies.
    - A GLP-compliant two-generation reproductive toxicity study conducted according to OECD 416 was performed with Wistar rats (24/sex/dose group) provided diets containing p-toluenesulfonamide (99.9% purity) at 0, 1,000, 3,000, or 10,000 ppm (equivalent to 0, 52-78, 165-237, and 566-832 mg/kg/day for males and 0, 75-161, 232-499, and 733-1,631 mg/kg/day for females, respectively). The original parental animals (F0 generation) were treated for 10 weeks prior to mating until the end of the study, the F1 animals were exposed in utero through nursing, directly following weaning and for 10 weeks prior to mating until the end of the study, and the F2 animals were exposed in utero and throughout the lactation period. The animals were evaluated for clinical signs of toxicity, body weight, food and water consumption, sperm parameters, estrous cyclicity, reproductive indices, offspring viability indices, gross pathology, and histopathology. No treatment-related effects were observed on clinical signs of toxicity, estrous cyclicity, sperm parameters, reproductive performance, gross pathology, or histopathology of the parental animals. Decreased body weight and body weight gain were consistently observed in the mid and high dose groups for males and females in the F0 and F1 generations. No treatment-related effects were observed on offspring viability, clinical signs of toxicity, sexual maturation, gross pathology, or histopathology. Decreased body weights were observed for male and female F1 pups in the high dose group and male

and female F2 pups in the high dose group. F1 male pups exhibited a delay in balanoperputial separation (external sign of puberty in male rat) (108% of control) and F1 female pups exhibited a delay in vaginal opening (114% of control). The study authors identified a developmental LOAEL of 10,000 ppm (566-832 mg/kg/day for males and 733-1,631 mg/kg/day for females) based on decreased pup weight and delayed sexual maturation in the F1 pups and a reproductive NOAEL of 10,000 ppm (566-832 mg/kg/day for males and 733-1,631 mg/kg/day for females) based on the lack of effects to reproduction observed in the study.

- A GLP-compliant combined repeated dose toxicity study with reproduction/developmental toxicity screening conducted according to OECD 422 was performed with Sprague-Dawley rats (13/sex/dose group) administered oral doses of p-toluenesulfonamide (purity not specified) at 0, 120, 300, or 750 mg/kg/day. The males were dosed for 42 days and the females were dosed for 14 days prior to mating to postnatal day 3. The parental animals were evaluated for clinical signs of toxicity, body weight, estrous cyclicity, and reproductive performance. The offspring were evaluated for viability, clinical signs of toxicity body weight, gross pathology, and histopathology. No treatment-related effects were observed on mating performance or fertility. In the high dose group, 2/10 females had difficult deliveries and all of their offspring died by postnatal day 3. The duration of gestation, numbers of corpora lutea, implantations and resorptions, litter size, and sex distribution were not affected by treatment. No teratogenic effects were observed with treatment. The survival rate and body weights of offspring in the high dose group were significantly decreased relative to control values. The study authors identified reproductive and developmental LOAELs of 750 mg/kg/day based on the decrease survival and body weight of the offspring in the high dose group.

Endocrine Activity (E) Score (H, M, or L): DG
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Data Gap for endocrine disruption based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - No data were identified for this endpoint.

<u>Group II and II* Human Health Effects (Group II and II* Human)</u>
Note: Group II and Group II* endpoints are distinguished in the v 1.2 Benchmark system. For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints and test data for single or repeated exposures may be used. If data exist for single OR repeated exposures, then the endpoint is not considered a data gap. If data are available for both single and repeated exposures, then the more conservative value is used.

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M, or L): L

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for acute toxicity based on oral LD_{50} values of greater than 2,000 mg/kg/day for n-ethyl-o (or p)-toluenesulfonamide and the surrogate p-toluenesulfonamide. GreenScreen® criteria classify chemicals as a Low hazard for acute toxicity when oral LD_{50} values are greater than 2,000 mg/kg (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - ChemIDplus 2014
    - *Oral*: LD_{50} (rat) = 2,250 mg/kg
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - *Oral*: LD_{50} (Wistar rat) = 2,330 mg/kg (OECD 401)
    - *Oral*: LD_{50} (Sprague-Dawley rat) = greater than 2,000 mg/kg (GLP-compliant, OECD 401)

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)

***Group II Score (single dose)* (vH, H, M, or L): L**

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for systemic toxicity (single dose) based on the lack of systemic effects in animals that survived to the scheduled sacrifice in an acute oral toxicity study of the surrogate p-toluenesulfonamide. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (single dose) when negative results, no structural alerts, and no GHS classification are available (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - *Oral*: No systemic toxicity data were presented for the study that identified an oral LD_{50} of 2,330 mg/kg in rats.
    - *Oral*: In the study that identified an oral LD_{50} value of greater than 2,000 mg/kg for rats, decreased activity and staggering gait were observed shortly after dosing at 889 to 3,000 mg/kg. Prone posture was observed at 1,333 and 2,000 mg/kg. Additional clinical signs of toxicity observed at 2,000 or 3,000 mg/kg included piloerection, lacrimation, pallor, reduced respiration, reduced pinna reflex, paralysis of the hind limbs, no reaction to external stimuli, closed eyes, decreased body surface temperature, and blood in urine. Decreased body weight was observed in the few animals that died at 2,000 or 3,000 mg/kg. No gross pathological effects were observed in animals that survived to the scheduled sacrifice. Reddened lungs, hyperemia of the jejunum adhesion, plaque hemorrhage of the thymus, and hematin of the gastric mucosa were observed.

***Group II* Score (repeated dose)* (H, M, or L): L**

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for systemic toxicity (repeated dose) based on an oral NOAEL of 100 mg/kg/day for n-ethyl-o (or p)-toluenesulfonamide and oral NOAELs

of 248-255 mg/kg/day for the surrogate p-toluenesulfonamide. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when oral LOAELs are greater than 100 mg/kg/day (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.
    - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
    - U.S. EPA 2006
        - *Oral*: A GLP-compliant subchronic repeated dose toxicity test conducted according to OECD 408 was performed with male and female Wistar rats (number not specified) administered oral doses of n-ethyl-o (or p)-toluenesulfonamide (purity not specified) at 0, 25, 100, or 400 mg/kg/day via gavage for 90 days. The animals were evaluated for clinical signs of toxicity, hematology, clinical chemistry, gross pathology, and histopathology. In the high dose group, salivation, lethargy, flat posture, and uncoordinated movements were observed within 5-10 minutes of dosing. Animals in the low and mid dose groups also exhibited these clinical signs but at a lower frequency and severity. These signs did not increase with frequency or severity within the same dose group as the study progressed. High dose group males and females exhibited increased albumin, total protein, and cholesterol levels; increased potassium and calcium levels were observed in high dose females only. No gross pathological findings were observed with treatment. The following organ weight changes were observed with treatment: the absolute liver weights increased in high dose males and mid and high dose females, the relative liver weights increased in high dose males and females of all dose groups, increased absolute kidney weights were observed in high dose females, and increased relative kidney weights were observed in high dose males and mid and high dose females. Cortical hyaline droplets were observed in the kidneys of mid and high dose males, and hyaline casts and corticomedullary tubular basophilia were observed in high dose males. Diffuse midzonal/centrilobular hypertrophy was observed in the livers of high dose females. The study authors considered the hypertrophy observed in the livers of high dose females to be an adaptive physiological response to xenobiotic exposure. They also concluded that the cortical hyalaine droplets observed in male kidneys were indicative of the accumulation of alpha-2u-globulin, an effect that is not relevant for human health. ToxServices identified a NOAEL and LOAEL of 100 and 400 mg/kg/day, respectively, based on the corticomedullary tubular basophilia observed in males of the high dose group.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
    - ECHA 2014
        - *Oral*: A GLP-complaint subchronic repeated dose toxicity study conducted in a manner similar to OECD 409 was performed with Beagle dogs (4/sex/dose group) provided diets containing p-toluenesulfonamide (99.9% purity) at 0, 1,000, 3,500, or 8,000 ppm (equivalent to 0, 30, 133, and 260 mg/kg/day for males and 0, 36, 114, and 255 mg/kg/day for females, respectively) for 90 days. The animals were evaluated for clinical signs of toxicity, body weight, food consumption, hematology, clinical chemistry, urinalysis, gross pathology, and histopathology. No treatment-related effects were observed on these parameters and the authors identified a NOAEL of 255 mg/kg/day.

- *Oral*: A GLP-compliant subchronic repeated dose toxicity study conducted in a manner similar to OECD 408 was performed with Wistar Han, Crl:WI(han) rats (10/sex/dose group) provided diets containing p-toluenesulfonamide (99.9% purity) at 0, 1,000, 3,000, or 10,000 ppm (equivalent to 0, 70, 214, and 738 mg/kg/day for males and 0, 80, 248, and 795 mg/kg/day for females, respectively) for at least 90 days. The animals were evaluated for clinical signs of toxicity, body weight, food consumption, hematology, clinical chemistry, gross pathology, and histopathology. No treatment-related effects were observed on clinical signs of toxicity, food consumption, hematology, clinical chemistry, organ weights, or gross pathology. The body weight and body weight gains of high dose males and females were reduced with treatment relative to controls. In the high dose group, 2/10 males exhibited a minimal degree of hyperplasia of the urothelium of the urinary bladder. The study authors identified a NOAEL and LOAEL of 248 and 738 mg/kg/day, respectively, based on the decreased body weight and body weight gain, and increased incidence of urothelial hyperplasia.

Neurotoxicity (N)

***Group II Score (single dose)* (vH, H, M, or L): H**

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of High for neurotoxicity (single dose) based on the effects to the nervous system observed following single oral doses of 2,000 mg/kg for the surrogate p-toluenesulfonamide. GreenScreen® criteria classify chemicals as a High hazard for neurotoxicity (single dose) when neurotoxic effects are observed at 300 to 2,000 mg/kg (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - *Oral*: No neurotoxicity data were presented for the study that identified an oral LD_{50} of 2,330 mg/kg in rats.
    - *Oral*: In the study that identified an oral LD_{50} value of greater than 2,000 mg/kg for rats, clinical signs of toxicity observed at 2,000 or 3,000 mg/kg included reduced pinna reflex, paralysis of the hind limbs, and a lack of reaction to external stimuli.

***Group II* Score (repeated dose)* (H, M, or L): L**

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for neurotoxicity (repeated dose) based on the lack of neurotoxicity observed in repeated dose toxicity studies of n-ethyl-o (or p)-toluenesulfonamide and the surrogate p-toluenesulfonamide. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (repeated dose) when negative data, no structural alerts, and no GHS classification are available (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006, 2014).

- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
    - U.S. EPA 2006
        - *Oral*: A GLP-compliant subchronic repeated dose toxicity test conducted according to OECD 408 was performed with male and female Wistar rats (number not specified) administered oral doses of n-ethyl-o (or p)-toluenesulfonamide (purity not specified) at 0, 25, 100, or 400 mg/kg/day via gavage for 90 days. The animals were evaluated in a functional observational battery (FOB) and motor activity test, and histopathology was performed on neuronal tissues. No treatment-related effects were observed on these parameters. ToxServices identified a neurotoxicity NOAEL of 400 mg/kg/day based on the lack of effects on neurobehavioral performance and neurological tissues.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
    - ECHA 2014
        - *Oral*: A GLP-compliant subchronic repeated dose toxicity study conducted in a manner similar to OECD 408 was performed with Wistar Han, Crl:WI(han) rats (10/sex/dose group) provided diets containing p-toluenesulfonamide (99.9% purity) at 0, 1,000, 3,000, or 10,000 ppm (equivalent to 0, 70, 214, and 738 mg/kg/day for males and 0, 80, 248, and 795 mg/kg/day for females, respectively) for at least 90 days. The animals were evaluated for grip strength, motor activity, hearing ability, pupillary reflex, and static righting reflex. No treatment-related effects were observed on these parameters. ToxServices identified a neurotoxicity NOAEL of 738 mg/kg/day based on the lack of neurobehavioral effects observed in this study at up to the highest dose tested.

Skin Sensitization (SnS) Group II* Score (H, M, or L): L
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for skin sensitization based on negative findings in a mouse local lymph node assay using the surrogate. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate data are available and negative, there are no structural alerts, and they are not GHS classified (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.
    - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide (CAS# 8047-99-2)
    - No data were identified.
- Surrogate: Toluene-4-Sulphonamide (CAS# 70-55-3)
    - ECHA 2014
        - Toluene-4-sulphonamide was not sensitizing in a GLP-compliant mouse local lymph node assay conducted according to OECD Guideline 429 in female CBA mice (4/dose). Mice were treated with 10, 25, or 50% (w/v) toluene-4-sulphonamide on the dorsal surface of each ear for three consecutive days. The authors reported a stimulation index less than three, indicating toluene-4-sulphonamide was not sensitizing.

Respiratory Sensitization (SnR) Group II* Score (H, M, or L): DG
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Data Gap for respiratory sensitization based on the lack of data identified for this endpoint.

- Authoritative and Screening Lists
    - *Authoritative:* Not listed on any authoritative lists for this endpoint.

- *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - No data were identified for this endpoint.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M, or L): L

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for skin irritation/corrosivity based on the findings of an acute dermal irritation study using the surrogate. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when adequate data are available and negative, there are no structural alerts, and they are not GHS classified (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - Toluene-4-sulphonamide was not irritating in an acute dermal irritation study in rabbits. Toluene-4-sulphonamide (0.5 g) was applied to intact and abraded skin of New Zealand white rabbits (6 animals with intact and 6 animals with abraded skin) under occlusive conditions for 24 hours. Dermal irritation was evaluated at 24 and 72 hours after the start of the exposure. There was no difference in dermal irritation between animals with intact and abraded skin. Treatment produced minimal irritation in rabbits with a mean erythema score of 0.3 and mean edema score of 0. The erythema was not reversible within 72 hours. These effects do not warrant a GHS classification.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M, or L): M

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Moderate for eye irritation/corrosivity based on findings in an acute eye irritation study using the surrogate. GreenScreen® criteria classify chemicals as a Moderate hazard for eye irritation/corrosivity when classified as GHS Category 2B (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide, CAS #8047-99-2
  - No data were identified for this endpoint.
- Surrogate: p-Toluenesulfonamide, CAS #70-55-3
  - ECHA 2014
    - Toluene-4-sulphonamide was not irritating in an acute eye irritation study in rabbits. Toluene-4-sulphonamide (0.1 g) was instilled into one eye of six New Zealand White rabbits. Ocular irritation was assessed at 24, 48, and 72 hours and 7 days after instillation. Treatment produced slight irritation with a mean conjunctivae redness score of 1 in three of the six treated animals. Conjunctivae redness was fully reversible in two of the three affected animals after 7 days.
- Based on the weight of the evidence, a score of Moderate was assigned. Mild eye irritation was reported in an acute ocular irritation study using the surrogate. Following gradings at 24, 48, and 72

hours, three of the six treated animals had mean conjunctivae redness scores of 1. The conjunctivae redness was fully reversible within 7 days in two of the three affected animals. The animals were only observed for 7 days; therefore, it is unknown if the conjunctivae redness was fully reversible in the last rabbit within 21 days. As the conjunctivae redness was fully reversible in two of the three affected animals within 7 days, ToxServices classified toluene ethylsulfonamide as GHS Category 2B.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): M

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Moderate for acute aquatic toxicity based on a measured EC_{50} for the surrogate. GreenScreen® criteria classify chemicals as a Moderate hazard for acute aquatic toxicity when the L/EC_{50} values are between 10 and 100 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide (CAS# 8047-99-2)
  - No measured data were identified for this endpoint.
  - U.S. EPA 2012a (see Appendix E)
    - 96h LC_{50} (fish) = 73.184 mg/L
    - 96h LC_{50} (daphnia) = 85.370 mg/L
    - 96h EC_{50} (algae) = 2.24 mg/L
- Surrogate: p-Toluenesulfonamide (CAS# 70-55-3)
  - ECHA 2014
    - 96h LC_{50} (*Salmo gairdneri*, rainbow trout) = 102 mg/L
    - 96h LC_{50} (*Lepomis macrochirus,* bluegill sunfish) = 370 mg/L
  - UNEP Undated
    - 72h EC_{50} (*Selenastrum capricornutum*, algae) = 23 mg/L
    - 24h EC_{50} (*Daphnia magna,* water flea) = 150 mg/L
    - 48-72h LC_{50} (*Oryzias latipes,* Orange-red Killifish) = 435 mg/L
- Based on the weight of evidence, a score of Moderate was assigned. No measured data were identified for n-ethyl-o (or p)-toluenesulfonamide and the most conservative predicted L/EC_{50} value was 2.24 mg/L in algae. Measured data was identified for the surrogate, toluene-4-sulphonamide, with L/EC_{50} values between 23 and 435 mg/L. Based on the most conservative measured EC_{50} of 23 mg/L in algae, a score of Moderate was assigned.

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): *H*

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of High for chronic aquatic toxicity based on a predicted chronic toxicity value in fish. GreenScreen® criteria classify chemicals as a High hazard for chronic aquatic toxicity when the chronic toxicity values are between 0.1 and 1 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* Not listed on any authoritative lists for this endpoint.
  - *Screening:* Not listed on any screening lists for this endpoint.
- Toluene Ethylsulfonamide (CAS# 8047-99-2)
  - No measured data were identified for this endpoint.
  - U.S. EPA 2012a (see Appendix E)
    - ChV (fish) = 0.116 mg/L
    - ChV (daphnia) = 4.408 mg/L

        - ChV (algae) = 1.996 mg/L
- Surrogate: p-Toluenesulfonamide (CAS# 70-55-3)
    - UNEP Undated
        - 21-day NOEC (*Daphnia magna*, water flea) = 47 mg/L
- Based on the weight of evidence, a score of High was assigned. No measured data were identified for n-ethyl-o (or p)-toluenesulfonamide. The most conservative predicted chronic toxicity value is 0.116 mg/L in fish. According to GreenScreen® criteria, a score of High is warranted if the chemical has chronic toxicity values between 0.1 and 1 mg/L. A measured 21 day NOEC of 47 mg/L in daphnia was identified for the surrogate. However, no chronic toxicity values were identified for fish or algae. Therefore, a score of High was assigned based on the most conservative modeled chronic toxicity value of 0.116 mg/L. Confidence in this endpoint was reduced due to the use of modeling.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): *H*
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of High for persistence based on the modeled half-life in soil. GreenScreen® criteria classify chemicals as a High hazard for persistence when the half-life in soil is between 60 and 180 days (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* not listed on any authoritative lists for this endpoint.
    - *Screening:* not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide (CAS# 8047-99-2)
    - No measured data were identified for this endpoint.
    - U.S. EPA 2012b
        - The BIOWIN modeling Ready Biodegradable Predictor indicates that n-ethyl-o (or p)-toluenesulfonamide is not expected to be readily biodegradable. Fugacity modeling predicts 77.5% will partition to soil with a half-life of 75 days, 21.4% will partition to water with a half-life of 37.5 days, and 0.871% will partition to air with a half-life of 1.06 days (see Appendix F).
- Surrogate: p-Toluenesulfonamide (CAS# 70-55-3)
    - ECHA 2014
        - Toluene-4-sulphonamide was readily biodegradable in a GLP-compliant OECD 301 D closed bottle test. Toluene-4-sulphonamide was 86% and 45% degraded after 28 days for the lowest (2 mg/L) and highest (4 mg/L) concentrations, respectively.
        - Toluene-4-sulphonamide was readily biodegradable in an OECD 301 D closed bottle test with 73% degraded after 10 days.
    - UNEP Undated
        - Toluene-4-sulphonamide was not readily biodegradable in an OECD 301 C MITI (I) test with 3% degraded after 28 days.
- Based on the weight of evidence, a score of High was assigned. No measured data was identified for n-ethyl-o (or p)-toluenesulfonamide. Fugacity modeling predicts that it will partition primarily to soil with a half-life of 75 days. When the major compartment is soil, GreenScreen® criteria specify a score of High if the chemical has a half-life between 60 and 180 days. Mixed results were identified for the surrogate. Two closed bottle tests (OECD 301 D) reported it was readily biodegradable while a MITI (I) test (OECD 301 C) indicated that it is not readily biodegradable. The surrogate toluene-4-sulphonamide is water soluble (3g/L) and not volatile (vapor pressure = 0.000286 Pa at 20 ºC) (ECHA 2014). The OECD 301 C test is most applicable to poorly soluble

substances that are or are not volatile while the OECD 301 D test is applicable to volatile substances that are or are not soluble. Neither OECD 301 C nor OECD 301 D is applicable to toluene-4-sulphonamide because it is soluble but not volatile. Therefore, ToxServices did not consider these studies for the classification of this endpoint. A score of High was assigned based on the estimated half-life of toluene ethylsulfonamide in soil. Confidence in this endpoint was reduced due to the use of modeling.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vL
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Very Low for bioaccumulation based on a measured log K_{ow} for the surrogate and estimated BCF values for the surrogate and n-ethyl-o (or p)-toluenesulfonamide. GreenScreen® criteria classify chemicals as a Very Low hazard for bioaccumulation when the BCF is less than 100 and the log K_{ow} less than 4 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists for this endpoint.
  - *Screening:* not listed on any screening lists for this endpoint.
- Toluene Ethylsulfonamide (CAS# 8047-99-2)
  - No measured data were identified for this endpoint.
  - U.S. EPA 2012b
    - BCFBAF predicts a BCF of 7.982 based on a log K_{ow} of 1.87 (estimated), indicating this chemical is not likely to bioaccumulate because the BCF is less than 100 based on a log K_{ow} less than 4 (see Appendix F).
- Surrogate: p-Toluenesulfonamide (CAS# 70-55-3)
  - ECHA 2014
    - Log K_{ow} = 0.6 (GLP, OECD 117)
  - HSDB 2004
    - A BCF of 3 was estimated based on a log K_{ow} of 0.82, indicating this chemicals is not likely to bioaccumulate because the BCF is less than 100 based on a log K_{ow} less than 4.
- Based on the weight of evidence, a score of Very Low was assigned. No measured data were identified for n-ethyl-o (or p)-toluenesulfonamide. BCFBAF modeling predicted a BCF of 7.982 based on a log K_{ow} of 1.87, indicating it is not likely to bioaccumulate. The surrogate has a measured log K_{ow} of 0.6. In addition, a BCF of 3 was estimated based on a log K_{ow} of 0.82. These data support the modeled data for toluene ethylsulfonamide indicating it is not likely to bioaccumulate based on BCF values less than 100 and log K_{ow} values less than 4.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for reactivity based on the weight of evidence. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when they are not explosive and not reactive otherwise (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists for this endpoint.
  - *Screening:* not listed on any screening lists for this endpoint.
- Toluene Ethylsulfonamide (CAS# 8047-99-2)
  - UNITEX 2009
    - A material safety data sheet for n-ethyl-o (or p)-toluenesulfonamide states that it has a reactivity rating of 1 from the HMIS "Materials that are normally stable, but can

become unstable at high temperatures and pressures" and NFPA "Normally stable, but can become unstable at elevated temperatures and pressures".

- Surrogate: p-Toluenesulfonamide (CAS# 70-55-3)
  - ECHA 2014
    - Toluene-4-sulphonamide is not an oxidizing substance (GLP, EU Method A.17).
  - Sigma-Aldrich 2014
    - A material safety data sheet for p-toluenesulfonamide states that it has a reactivity rating of 0 from the HMIS "Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosive" and NFPA "Normally stable, even under fire exposure conditions, and is not reactive with water".
- Based on the weight of evidence, a score of Moderate was assigned. The HMIS and NFPA reactivity ratings for n-ethyl-o (or p)-toluenesulfonamide indicate that it is normally stable but may become unstable at high temperatures and pressures. As HMIS and NFPA reactivity ratings do not align with GreenScreen® guidance for assessing reactivity, data for the surrogate was used as supportive evidence for this endpoint. The surrogate is not oxidizing and its HMIS and NFPA reactivity ratings indicate that it is not self-reactive or explosive, which warrants a Low score. n-Ethyl-o (or p)-toluenesulfonamide and its surrogate have similar structures and are expected to have similar reactivity profiles. Therefore, a score of Low was assigned. Confidence in this endpoint was reduced due to the use of an MSDS.

Flammability (F) Score (vH, H, M, or L): L

n-Ethyl-o (or p)-toluenesulfonamide was assigned a score of Low for flammability based on its flash point and classification by HMIS and NFPA. GreenScreen® criteria classify chemicals as a Low hazard for flammability when they are not classified as flammable liquids per GHS (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists for this endpoint.
  - *Screening:* not listed on any screening lists for this endpoint.
- n-Ethyl-o (or p)-toluenesulfonamide (CAS# 8047-99-2)
  - NTP 1991
    - Flash point = greater than 93 ºC
  - UNITEX 2009
    - A material safety data sheet for n-ethyl-o (or p)-toluenesulfonamide states that it has a flammability rating of 1 from the HMIS "Materials that must be preheated before ignition will occur. Includes liquids, solids, and semi-solids having a flash point above 200 F (Class IIIB)" and NFPA "Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93 ºC (200 ºF)".
- Based on the information above stating that n-ethyl-o (or p)-toluenesulfonamide is nonflammable, ToxServices did not classify n-ethyl-o (or p)-toluenesulfonamide as a flammable chemical based on GHS criteria (UN 2013). GHS flammable liquids have flash points of no greater than 93°C.

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APPENDIX A: Hazard Benchmark Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	n-Ethyl-o (or p)-toluenesulfonamide	**8047-99-2**	*L*	**L**	**M**	**M**	DG	**L**	**L**	**L**	**H**	**L**	**L**	DG	**L**	**M**	**M**	*H*	*H*	**vL**	*L*	**L**

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	No	No	No	No	No		
2	No	No	Yes	No	Yes	No	No
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
n-Ethyl-o (or p)-toluenesulfonamide	2

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

Chemical Name	Final GreenScreen® Benchmark Score
n-Ethyl-o (or p)-toluenesulfonamide	2

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

APPENDIX C: Pharos Output for n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)

Search Results for '8047-99-2'

Companies (0) | Building Products (0) | Chemicals, Compounds, and Biobased Materials (0) | Signal Articles (0) | Certifications (0)

Companies

*There were no companies found that match the search term **8047-99-2**.*

Back to top

Building Products

*There were no products found that match the search term **8047-99-2**.*

Back to top

Chemicals, Compounds, and Biobased Materials

*There were no chemicals, compounds, or biobased materials found that match the search term **8047-99-2**.*

Back to top

Signal Articles

*There were no Signal articles found that match the search term **8047-99-2**.*

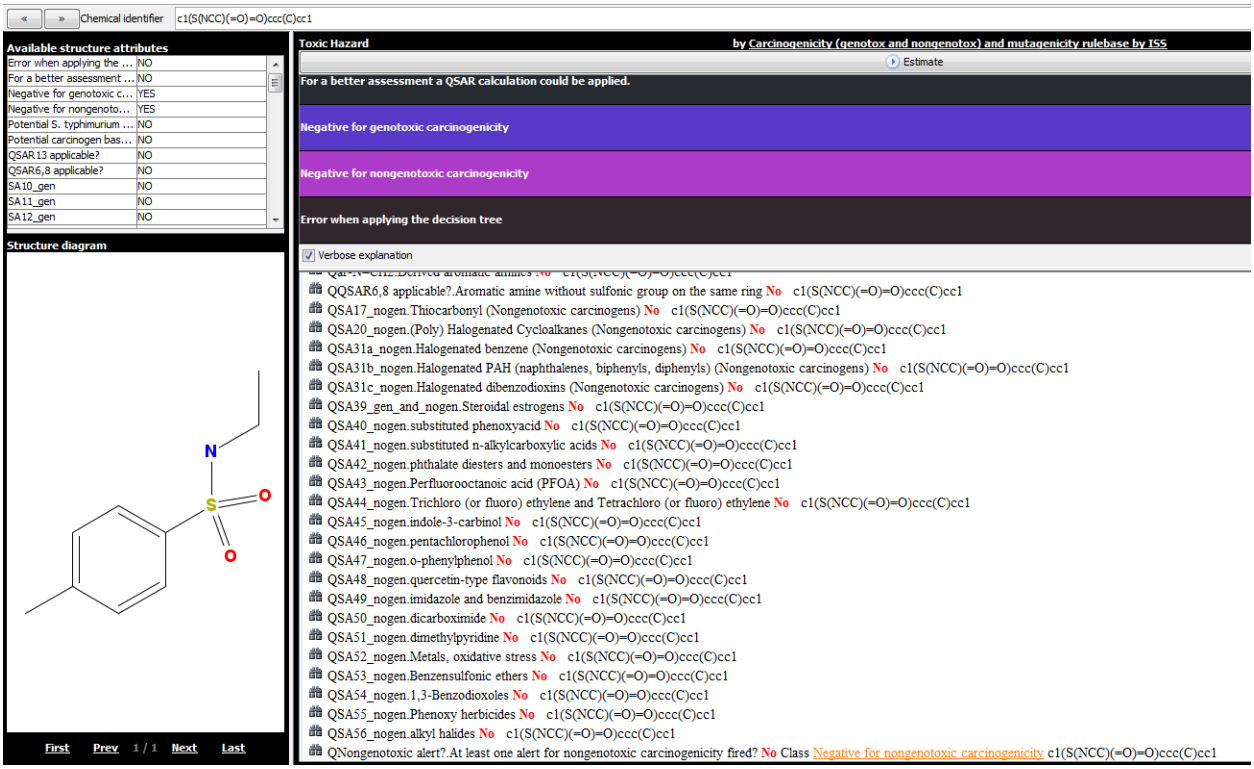
Back to top

Certifications

*There were no certifications found that match the search term **8047-99-2**.*

Back to top

APPENDIX D: ToxTree Carcinogenicity Results for n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)



APPENDIX E: ECOSAR Modeling Results for n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)

ECOSAR Version 1.11 Results Page

SMILES: c1(S(NCC)(=O)=O)ccc(C)cc1
CHEM:
CAS Num: 8047-99-2
ChemID1:
MOL FOR: C9 H13 N1 O2 S1
MOL WT: 199.27
Log K_{ow}: 1.875 (EPISuite K_{ow}win v1.68 Estimate)
Log K_{ow}: (User Entered)
Log K_{ow}: (PhysProp DB exp value - for comparison only)
Melt Pt: (User Entered for Wat Sol estimate)
Melt Pt: (deg C, PhysProp DB exp value for Wat Sol estimate)
Wat Sol: 1106 (mg/L, EPISuite WSK_{ow}win v1.43 Estimate)
Wat Sol: (User Entered)
Wat Sol: (PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log K_{ow}: 1.875 (EPISuite K_{ow}win v1.68 Estimate)
Wat Sol: 1106 (mg/L, EPISuite WSK_{ow}win v1.43 Estimate)

Available Measured Data from ECOSAR Training Set

No Data Available

ECOSAR v1.1 Class-specific Estimations

Amides

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Amides	: Fish	96-hr.	LC50	73.184
Amides	: Daphnid	48-hr.	LC50	85.370
Amides	: Green Algae	96-hr.	EC50	2.240
Amides	: Fish		ChV	0.116
Amides	: Daphnid		ChV	4.408
Amides	: Green Algae		ChV	1.996
Amides	: Fish (SW)	96-hr.	LC50	64.560
Amides	: Mysid (SW)	96-hr.	LC50	3.924

Neutral Organic SAR	: Fish	96-hr.	LC50	212.159
(Baseline Toxicity)	: Daphnid	48-hr.	LC50	119.079
	: Green Algae	96-hr.	EC50	84.556
	: Fish	ChV		20.456
	: Daphnid	ChV		11.244
	: Green Algae	ChV		21.580

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogK_{ow} Cut-Offs

If the log K_{ow} of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Amides :

Maximum LogK_{ow}: >8.5 (LC50)
Maximum LogK_{ow}: >8.0 (EC50,ChV)

Baseline Toxicity SAR Limitations:

Maximum LogK_{ow}: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogK_{ow}: 6.4 (Green Algae EC50)
Maximum LogK_{ow}: 8.0 (ChV)

APPENDIX F: EPISuite Modeling Results for n-Ethyl-o (or p)-toluenesulfonamide (CAS #8047-99-2)

CAS Number: 8047-99-2
SMILES: c1(S(NCC)(=O)=O)ccc(C)cc1
CHEM:
MOL FOR: C9 H13 N1 O2 S1
MOL WT: 199.27
---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log K_{ow} (octanol-water): ------
Boiling Point (deg C): ------
Melting Point (deg C): ------
Vapor Pressure (mm Hg): ------
Water Solubility (mg/L): ------
Henry LC (atm-m^3/mole): ------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (K_{ow}WIN v1.68 estimate) = 1.87

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 323.83 (Adapted Stein & Brown method)
Melting Pt (deg C): 96.48 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 0.000111 (Modified Grain method)
VP (Pa, 25 deg C): 0.0147 (Modified Grain method)
Subcooled liquid VP: 0.000546 mm Hg (25 deg C, Mod-Grain method)
: 0.0727 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log K_{ow} (WSK_{ow} v1.42):
Water Solubility at 25 deg C (mg/L): 1106
log K_{ow} used: 1.87 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 760.5 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Amides

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method: 1.36E-006 atm-m^3/mole (1.38E-001 Pa-m^3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 2.631E-008 atm-m^3/mole (2.666E-003 Pa-m^3/mole)
VP: 0.000111 mm Hg (source: MPBPVP)

WS: 1.11E+003 mg/L (source: $WSK_{ow}WIN$)

Log Octanol-Air Partition Coefficient (25 deg C) [K_{oa}WIN v1.10]:
Log K_{ow} used: 1.87 (K_{ow}Win est)
Log K_{aw} used: -4.255 (HenryWin est)
Log K_{oa} (K_{oa}WIN v1.10 estimate): 6.125
Log K_{oa} (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.7073
Biowin2 (Non-Linear Model): 0.6805
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.6840 (weeks-months)
Biowin4 (Primary Survey Model): 3.4917 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.2435
Biowin6 (MITI Non-Linear Model): 0.1202
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.0290
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.0728 Pa (0.000546 mm Hg)
Log K_{oa} (K_{oa}win est): 6.125
Kp (particle/gas partition coef. ($m^3/\mu g$)):
Mackay model: 4.12E-005
Octanol/air (K_{oa}) model: 3.27E-007
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 0.00149
Mackay model: 0.00329
Octanol/air (K_{oa}) model: 2.62E-005

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 10.0778 E-12 cm^3/molecule-sec
Half-Life = 1.061 Days (12-hr day; 1.5E6 OH/cm^3)
Half-Life = 12.736 Hrs.
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
0.00239 (Junge-Pankow, Mackay avg)
2.62E-005 (K_{oa} method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (K_{oc}WIN v2.00):
K_{oc}: 177 L/kg (MCI method)

Log K_{oc}: 2.248 (MCI method)
K_{oc}: 125.6 L/kg (K_{ow} method)
Log K_{oc}: 2.099 (K_{ow} method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 0.904 (BCF = 8.014 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -0.4739 days (HL = 0.3358 days)
Log BCF Arnot-Gobas method (upper trophic) = 0.902 (BCF = 7.982)
Log BAF Arnot-Gobas method (upper trophic) = 0.902 (BAF = 7.982)
log K_{ow} used: 1.87 (estimated)

Volatilization from Water:
Henry LC: 1.36E-006 atm-m^3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 609.1 hours (25.38 days)
Half-Life from Model Lake: 6764 hours (281.8 days)

Removal in Wastewater Treatment:
Total removal: 2.22 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 2.05 percent
Total to Air: 0.08 percent
(using 10000 hr. Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	0.871	25.5	1000
Water	21.4	900	1000
Soil	77.5	1.8e+003	1000
Sediment	0.227	8.1e+003	0

Persistence Time: 998 hr.

Sources to Check for GreenScreen® Hazard Assessment

Note: For a GreenScreen® Hazard Assessment, data queries should be initially limited to the following references. If data gaps exist after these references have been checked, additional references may be utilized.

U.S. EPA High Production Volume Information System (HPVIS):
http://www.epa.gov/hpvis/index.html

UNEP OECD Screening Information Datasets (SIDS):
http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html

OECD Existing Chemicals Database: http://webnet.oecd.org/hpv/ui/SponsoredChemicals.aspx

European Chemical Substances Information System IUCLID Chemical Data Sheets:
http://esis.jrc.ec.europa.eu/index.php?PGM=dat

National Toxicology Program: http://ntp.niehs.nih.gov/

International Agency for the Research on Cancer:
http://monographs.iarc.fr/ENG/Classification/index.php

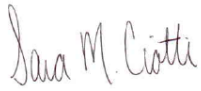
Human and Environmental Risk Assessment (HERA) on ingredients of household cleaning products:
http://www.heraproject.com/RiskAssessment.cfm

European Chemicals Agency (ECHA) REACH Dossiers: http://echa.europa.eu/

Licensed GreenScreen® Profilers

n-Ethyl-o (or p)-toluenesulfonamide GreenScreen® Evaluation Prepared by:

Zach Guerrette, Ph.D.
Toxicologist
ToxServices LLC



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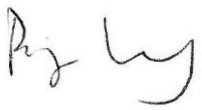
n-Ethyl-o (or p)-toluenesulfonamide GreenScreen® Evaluation QC'd by:



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