Development Support Document
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Pentenes

CAS Registry Numbers:
1-pentene: 109-67-1
c-2-pentene: 627-20-3
t-2-pentene: 646-04-8

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Chapter 1 Summary Tables

Table 1 provides a summary of health- and welfare-based values resulting from an acute and chronic evaluation of pentene. Summary information on the physical/chemical parameters of pentene can be found in Table 2.

Table 1. Health- and Welfare-Based Values

Short-Term Value	Concentration	Notes
Acute ReV	---	A generic ESL was developed since the minimum database for an acute ReV was not met.
$^{acute}ESL_{generic}$ [1 h]	7,500 µg/m^3 (2,600 ppb)* **Short-term ESL for Air Permit Reviews of c-2 pentene and t-2 pentene**	Tier II generic ESL
$^{acute}ESL_{odor}$	290 µg/m^3 (100 ppb)* **Short-term ESL for Air Permit Reviews of 1-pentene**	50% odor detection threshold **NOTE:** applies only to 1-pentene
$^{acute}ESL_{veg}$	---	No data found
Long-Term Value	**Concentration**	**Notes**
Chronic ReV	---	The minimum database for development of a chronic ReV was not met.
$^{chronic}ESL_{linear(nc)}$ $^{chronic}ESL_{nonlinear(nc)}$	---	No data found
$^{chronic}ESL_{linear(c)}$ $^{chronic}ESL_{nonlinear(c)}$	---	No data found
$^{chronic}ESL_{veg}$	---	No data found

*Values that may be used for evaluation of air monitoring data

Abbreviations:
ppb, parts per billion; **µg/m^3**, micrograms per cubic meter; **h**, hour; **ESL**, Effects Screening Level; **ReV**, Reference Value; ^{acute}**ESL$_{generic}$**, acute health-based ESL based on generic threshold of concern approach; ^{acute}**ESL$_{odor}$**, acute odor-based ESL; ^{acute}**ESL$_{veg}$**, acute vegetation-based ESL; ^{chronic}**ESL$_{nonlinear(nc)}$**, chronic health-based ESL for nonlinear dose-response noncancer effects; ^{chronic}**ESL$_{linear(c)}$**, chronic health-based ESL for linear dose-response cancer effects; ^{chronic}**ESL$_{nonlinear(c)}$**, chronic health-based ESL for nonlinear dose-response cancer effects; and ^{chronic}**ESL$_{veg}$**, chronic vegetation-based ESL

Chemical Structure:

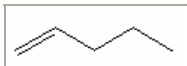
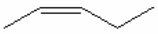
1-pentene	
trans-2-pentene	
cis-2-pentene	

Table 2. Chemical and Physical Data

Parameter	1-pentene	*cis*-2-pentene	*trans*-2-pentene	Reference
Molecular Formula	C_5H_{10}	C_5H_{10}	C_5H_{10}	HSDB (2002)
Molecular Weight	70.13	70.13	70.13	HSDB (2002)
Physical State	Liquid	Liquid	Liquid	HSDB (2002)
Color	Colorless	---	---	HSDB (2002)
Odor	Highly disagreeable	---	---	HSDB (2002)
CAS Registry Number	109-67-1	627-20-3	646-04-8	HSDB (2002)
Synonyms	α-amylene; α-n-amylene; 1-pentalyene; propylethylene	β-amylene-cis; cis-β-amylene; cis-β-N-amylene; cis-pentene; (Z)-2-pentene	β-amylene-trans; trans-β-amylene; trans-β-N-amylene; (E)-2-pentene; 2-trans-pentene	HSDB (2002)
Water Solubility	148 mg/L @ 25°C	203 mg/L @ 25°C	203 mg/L @ 25°C	HSDB (2002)
Log K_{ow} or P_{ow}	---	---	---	---
Vapor Pressure	635 mm Hg @ 25°C	495 mm Hg @ 25°C	506 mm Hg @ 25°C	HSDB (2002)
Relative Vapor Density	2.42	2.4	---	HSDB (2002)
Density	0.6405 @ 25°C	0.6554 @ 20°C	0.6431 @ 25°C	HSDB (2002)
Melting Point	-165.2°C	-151.4°C	-140.2°C	HSDB (2002)
Boiling Point	29.9°C	36.9°C	36.3°C	HSDB (2002)
Conversion Factors @ 25°C	1 μg/m^3 = 0.35 ppb 1 ppb = 2.87 μg/m^3	1 μg/m^3 = 0.35 ppb 1 ppb = 2.87 μg/m^3	1 μg/m^3 = 0.35 ppb 1 ppb = 2.87 μg/m^3	Toxicology Section

Chapter 2 Major Uses or Sources

According to the Hazardous Substances Data Bank (HSDB 2002), 1-pentene is primarily used in organic synthesis as a blending agent for high octane motor fuel and in pesticide formulations. 2-pentene is used as a polymerization inhibitor in organic synthesis.

Chapter 3 Acute Evaluation

3.1 Health-Based acute ESL

Well-conducted studies are available for petroleum distillate blending streams. However, the distillate is a mixture of compounds, making it impossible to differentiate the effects of specific chemicals. One study evaluating hemoglobin and DNA adduct formation suggests decreasing toxicity with increasing carbon chain length (Eide 1995). However, this study does not provide an appropriate point of departure from which to develop a ReV. Therefore, the minimum database for estimating an acute ReV was not met, and procedures outlined in Section 3.6.2 *Tier II Generic ESL: Threshold of Concern and LC_{50} Data Approaches* were followed to estimate a Tier II generic ESL (TCEQ 2006). The following acute toxicity data were reported in the RTECS database (2006):

4 hr LC_{50} in rats = 175,000 mg/m^3
2 hr LC_{50} in mice = 180,000 mg/m^3

These concentrations that were shown to be lethal to 50% of the study specimens (LC_{50}) were used in the generic ESL development procedure. As stated in Section 2.8 of the ESL guidelines, a duration adjustment to 4 hr is required for the 2 hr LC_{50} data (TCEQ 2006). Since the mode of action (MOA) is unknown, default procedures discussed in TCEQ (2006) with n=1 were used to adjust exposure duration as follows:

$C_1 \times T_1 = C_2 \times T_2$

180,000 mg/m^3 x 2 hours = C_2 x 4 hours

$C_2 = 180{,}000 \times (2/4)$

C_2 = 90,000 mg/m^3

3.1.1 Threshold of Concern (TOC) Approach

Based on its vapor pressure of 635 mm Hg at 25°C (HSDB 2002), pentene was considered a vapor under the Globally Harmonized System of Classification and Labeling of Chemicals (UN 2005; TCEQ 2006). Pentene was classified in Category 5 under the Threshold of Concern (TOC) approach, based on the LC_{50} values, which are both greater than 20,000 mg/m^3. The TOC generic ESL for Category 5 is 1,000 µg/m^3**.**

3.1.2 LC_{50} Data Approach

A 4-hr inhalation exposure study in rats determined the LC_{50} to be 175,000 mg/m^3 or 175,000,000 µg/m^3. Grant et al. (2007) determined a NOAEL to LC_{50} ratio of 8.3 x 10^{-5}. This factor is multiplied by LC_{50} values that have been adjusted to 4 hours to estimate a conservative generic ESL below which no

appreciable human health risks would be expected to occur. When the LC_{50} for pentene is multiplied by 8.3×10^{-5}, the generic ESL is 14,500 µg/m^3 (5,060 ppb). A 2-hr inhalation exposure study in mice reported an LC_{50} value of 180,000 mg/m^3. Adjusting to a 4-hr duration yields an LC_{50} value of 90,000 mg/m^3 or 90,000,000 µg/m^3. If the LC_{50} is multiplied by 8.3×10^{-5}, the generic ESL is 7,500 µg/m^3 (2,600 ppb).

3.1.3 Final Tier II Generic ESL

While confidence in these LC_{50} values is low, the chemical structure of pentene indicates that it is relatively non-toxic. The Cramer classification scheme is a well-known approach for classifying chemical toxicity based on chemical structure and recognized pathways for metabolic activation and deactivation (Cramer 1978). Although this classification scheme was originally developed for oral toxicity, it does contribute to the weight of evidence to indicate whether the chemical structure presents a potential concern for toxicity. The Cramer classification scheme places substance in one of three classes. Class I substances have simple chemical structure with known metabolic pathways that produce innocuous end products. Class II contains substances with chemical structures associated with intermediate toxicity. Class III substances possess structural features associated with significant toxicity. Pentene is classified as Cramer Class I (Toxtree v1.20). Based on the weight of evidence, a Tier II generic ESL of 7,500 µg/m^3 (2,600 ppb) was identified as the health-based acute ESL.

Toxicity data are unavailable for other isomers of pentene. However, the chemical and physical properties of these isomers are quite similar to 1-pentene. Therefore, this generic ESL will be applied to all isomers. This generic ESL will also be utilized during evaluation of air monitoring data in lieu of a ReV until data are available to derive a pentene-specific ReV, or a sufficient database of related chemicals has been developed under the new ESL guidelines to utilize a relative toxicity approach.

3.2. Welfare-Based Acute ESLs

3.2.1 Odor Perception

The Japanese Ministry of the Environment is listed as a source of information for odor thresholds in Appendix B of the ESL Guidelines (TCEQ 2006). The 50% odor detection threshold for 1-pentene determined by the triangular odor bag method was 0.10 ppm (Nagata 2003). Therefore, the acute, odor-based ESL for 1-pentene is 290 µg/m^3 (100 ppb). Odor data are unavailable for other isomers of pentene. Nagata et al. (2003) describe wide variation in the odor threshold between isomers of other substances. Therefore, unlike the acute, generic ESL, which is applied to all isomers of pentene, the odor threshold is specific for 1-pentene.

3.2.2 Vegetation Effects

No acute vegetative studies were identified for any isomers of pentene.

3.3. Short-term ESLs and Values for Air Monitoring Evaluation

For 1-pentene, this acute evaluation resulted in the derivation of the following acute values:

- $^{acute}ESL_{odor}$ = 290 µg/m^3 (100 ppb)
- $^{acute}ESL_{generic}$ = 7,500 µg/m^3 (2,600 ppb)

The short-term ESL for air permit evaluations of 1-pentene is 290 µg/m^3 (100 ppb) (Table 1). For evaluation of air monitoring data, the $^{acute}ESL_{odor}$ of 290 µg/m^3 (100 ppb), and the $^{acute}ESL_{generic}$ of 7,500 µg/m^3 may be used (2,600 ppb) (Table 1).

For c-2-pentene and t-2-pentene, this acute evaluation resulted in the derivation of the following acute value:

- $^{acute}ESL_{generic}$ = 7,500 µg/m^3 (2,600 ppb)

The short-term ESL for air permit evaluations is 7,500 µg/m^3 (2,600 ppb). The $^{acute}ESLs_{generic}$ value of 7,500 µg/m^3 (2,600 ppb) is also used in the evaluation of air monitoring data (Table 1).

Chapter 4 Chronic Evaluation

4.1. Non-carcinogenic Potential

No studies were available describing the potential chronic toxicity of any isomer of pentene. According to the ESL guidelines, if the minimum database requirements are not met, then a chronic ESL and ReV are not developed (TCEQ 2006).

4.2. Carcinogenic Potential

There are no studies indicating that pentene has carcinogenic potential.

4.3. Welfare-Based Chronic ESL

4.3.1 Vegetation Effects

No chronic vegetative studies were identified for any isomers of pentene.

Chapter 5 References

5.1 References Cited in the Development Support Document

Cramer, GM, RA Ford, and RL Hall. 1978. Estimation of toxic hazard – a decision tree approach. *Food Cosmet Toxicol* 16:255-76.

Grant, RL, BJ Kadlubar, NK Erraguntla, and M Honeycutt. 2007. Evaluation of acute inhalation toxicity for chemicals with limited toxicity information. *Regu Toxicol Pharmacol* 47:261-73.

Hazardous Substances Data Bank (HSDB). 2002 update. United States National Library of Medicine, http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB, accessed May 4, 2007.

Nagata, Y. 2003. Measurement of odor threshold by triangle odor bag method. Odor Measurement Review, Japan Ministry of the Environment. 118-27.

Registry of Toxic Effects of Chemical Substances (RTECS). 2006 update. Canadian Centre for Occupational Health and Safety, http://ccinfoweb.ccohs.ca/rtecs/search.html, accessed May 4, 2007.

Texas Commission on Environmental Quality (TCEQ). 2006. Guidelines to develop effects screening levels, reference values, and unit risk factors. Chief Engineer's Office. RG-442.

United Nations (UN). 2005. Globally harmonized system of classification and labeling of chemicals (GHS) First revised edition. ST/SG/AC.10/30/Rev.1 United Nations, New York and Geneva.

5.2 References of Other Studies Reviewed by the TS

Bui, QQ, DM Burnett, RJ Breglia, FJ Koschier, ES Lapadula, PI Podhasky, CA Schreiner, and RD White. 1998. Toxicity evaluation of petroleum blending streams: Reproductive and developmental effects of a distillate from light alkylate naphtha. *J Toxicol Environ Health* 53:121-33.

Eide, I, R Hagemann, K Zahlsen, E Tareke, M Tornqvist, R Kumar, P Vodicka, and K Hemminki. 1995. Uptake, distribution, and formation of hemoglobin and DNA adducts after inhalation of C2-C8 1-alkenes (olefins) in the rat. *Carcinogenesis* 16:1603-09.

Lapin, C, Q Bui, R Breglia, F Koschier, P Podhasky, E Lapadula, R Roth, C Schreiner, R White, C Clark, R Mandella, and G Hoffman. 2001. Toxicity evaluation of petroleum blending streams: Inhalation subchronic toxicity/neurotoxicity study of a light catalytic cracked naphtha distillate in rats. *Int J Toxicol* 20:307-19.

Schreiner ,C, Q Bui, R Breglia, D Burnett, F Koschier, P Podhasky, and R White. 2000. Toxicity evaluation of petroleum blending streams: Reproductive and developmental effects of light catalytic reformed naphtha distillate in rats. *J Toxicol Environ Health* 60:169-84.

Schreiner, C, Q Bui, R Breglia, D Burnett, F Koschier, E Lapadula, P Podhasky, and R White. 2000. Toxicity evaluation of petroleum blending streams: Inhalation subchronic toxicity/neurotoxicity study of a light catalytic reformed naphtha distillate in rats. *J Toxicol Environ Health* 60:489-512.