

APPENDIX A**MRLS AND CANCER CLASSIFICATION FOR TPH COMPONENTS AND
WHOLE PRODUCTS**

MRLs listed in Table A-1 are found in Appendix A of the individual Toxicological Profile referenced. Appendix A of each profile describes the basis for ATSDR MRL's derivation and use and includes worksheets showing calculations used to derive each MRL.

APPENDIX A

Table A-1. Minimal Risk Levels and Cancer Classification for TPH Components and Whole Products^a

Chemical	MRL (inhalation)	MRL (oral)	IARC Cancer Classification ^b	EPA Cancer classification ^c
Automotive gasoline ^d	NA	NA	NA	NA
Benzene ^e	0.05 ppm (acute), 0.004 ppm (intermediate)	NA	Group 1	Group A
Ethylbenzene ^f	0.2 ppm (intermediate)	NA	NA	Group D
Fuel Oils ^g	0.02 mg/m ³ (acute, diesel fuels), 0.01 mg/m ³ (intermediate, kerosene)	NA	Group 2A: petroleum refining, occupational Group 2B: marine diesel fuels & residual fuel oils Group 3: jet fuels & distillate diesel fuels	NA
<i>n</i> -Hexane ^h	0.6 ppm (chronic)	NA	NA	Group D
Jet Fuels ⁱ	9 mg/m ³ (intermediate, JP-4) 3 mg/m ³ (intermediate, JP 5/8) 0.3 mg/m ³ (chronic, JP-7)	NA	Group 3	NA
Mineral-based Crankcase Oil ^j	NA	NA	NA	NA
Naphthalene ^k	0.002 ppm (chronic, naphthalene)	0.05 mg/kg/day (acute, naphthalene) 0.02 mg/kg/day (intermediate, naphthalene) 0.07 mg/kg/day (chronic, 1-methylnaphthalene)	Group 3	Group D
PAHs ^l	NA	0.6 mg/kg/day (intermediate, acenaphthene) 0.4 mg/kg/day (intermediate, fluoranthene & fluorene) 10 mg/kg/day (intermediate, anthracene)	Group 2A: benz(a)anthracene, benzo(a)pyrene Group 2B: benzo(b)fluoranthene, benzo(j)fluoranthene, ideno(1,2,3-c,d)pyrene Group 3: anthracene, benzo(g,h,i)perylene, & additional PAHs	Group B2: benz(a)anthracene, benzo(b)fluoranthene, benzo(a)pyrene, chrysene, dibenz(a,h)anthracene, indeno(1,2,3-c,d)pyrene Group D: acenaphthylene, anthracene, fluoranthene
Toluene ^m	3 ppm (acute) 1 ppm (chronic)	0.8 mg/kg/day (acute) 0.02 mg/kg/day (intermediate)	NA	Group D

APPENDIX A

Table A-1. Minimal Risk Levels and Cancer Classification for TPH Components and Whole Products^a (continued)

Chemical	MRL (inhalation)	MRL (oral)	IARC Cancer Classification ^b	EPA Cancer classification ^c
Xylenes ⁿ	1 ppm (acute, mixed xylenes) 0.7 ppm (intermediate, mixed xylenes) 0.1 ppm (chronic, mixed xylenes)	1 mg/kg/day (acute, p-xylene) 0.2 mg/kg/day (intermediate, mixed xylenes) 0.6 mg/kg/day (intermediate, m-xylene)	Group 3	Group D

NA = not available

- ^a MRLs listed in Table A-1 are found in Appendix A of the individual Toxicological Profile referenced. Appendix A of each profile describes the basis for ATSDR MRL's derivation and use and includes worksheets showing calculations used to derive each MRL.
- ^b IARC Cancer Classifications: Group 1: carcinogenic to humans, Group 2A: probably carcinogenic to humans, Group 2B: possibly carcinogenic to humans, Group 3: not classifiable as to its carcinogenicity to humans
- ^c EPA Cancer Classifications: Group A; known human carcinogen, Group B2: probable human carcinogen, Group C: possible human carcinogen, Group D; not classifiable as to its carcinogenicity to humans
- ^d ATSDR. 1995a. Toxicological profile for automotive gasoline. Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA. NTIS PB95-264206.
- ^e ATSDR. 1997a. Toxicological profile for benzene (update). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.
- ^f ATSDR. 1997b. Toxicological profile for ethylbenzene (draft for public comment). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.
- ^g ATSDR. 1995g. Toxicological profile for fuel oils. Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA. NTIS PB95-264222.
- ^h ATSDR. 1997c. Toxicological profile for hexane (draft for public comment). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.
- ⁱ ATSDR. 1995c. Toxicological profile for jet fuels (JP-4 and JP-7). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA. NTIS PB95-264230.
- ATSDR. 1998b. Toxicological profile for jet fuels (JP-5 and JP-8) (February 1998 draft final). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.
- ^j ATSDR. 1997e. Toxicological profile for mineral-based crankcase oil. Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.
- ^k ATSDR. 1995e. Toxicological profile for naphthalene (update). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.
- ^l ATSDR. 1995f. Toxicological profile for polycyclic aromatic hydrocarbons (PAHS) (update). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.
- ^m ATSDR. 1994. Toxicological profile for toluene (update). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA. TP-93/14.
- ⁿ ATSDR. 1995d. Toxicological profile for xylenes (update). Agency for Toxic Substances and Disease Registry, Public Health Service, U.S. Department of Health and Human Services, Atlanta, GA.

APPENDIX B

USER'S GUIDE

Chapter 1

Public Health Statement

This chapter of the profile is a health effects summary written in non-technical language. Its intended audience is the general public especially people living in the vicinity of a hazardous waste site or chemical release. If the Public Health Statement were removed from the rest of the document, it would still communicate to the lay public essential information about the chemical.

The major headings in the Public Health Statement are useful to find specific topics of concern. The topics are written in a question and answer format. The answer to each question includes a sentence that will direct the reader to chapters in the profile that will provide more information on the given topic.

Chapter 6

Tables and Figures for Fraction-Specific Critical Effects

Tables (6-1 through 6-11) and Figures (6-1 through 6-16) summarize health effects and illustrate graphically levels of exposure associated with those effects. These levels cover health effects observed at increasing dose concentrations and durations, differences in response by species, minimal risk levels (MRLs) to humans for noncancer end points, and EPA's estimated range associated with an upper-bound individual lifetime cancer risk of 1 in 10,000 to 1 in 10,000,000. Use these tables and figures for a quick review of the health effects and to locate data for a specific exposure scenario. The Critical Effects tables and Exposure Assessment figures in Chapter 6 should always be used in conjunction with the text. All entries in these tables and figures represent studies that provide reliable, quantitative estimates of No-Observed-Adverse-Effect Levels (NOAELs), Lowest-Observed-Adverse-Effect Levels (LOAELs), or Cancer Effect Levels (CELs).

Chapter 6 (Section 6.7)

Relevance to Public Health

The Relevance to Public Health section provides a health effects summary based on evaluations of existing toxicologic, epidemiologic, and toxicokinetic information. This summary is designed to present interpretive, weight-of-evidence discussions for human health end points by addressing the following questions.

- 1 . What effects are known to occur in humans?
- 2 . What effects observed in animals are likely to be of concern to humans?
- 3 . What exposure conditions are likely to be of concern to humans, especially around hazardous waste sites?

The carcinogenic potential of the profiled substance is qualitatively evaluated, when appropriate, using existing toxicokinetic, genotoxic, and carcinogenic data. ATSDR does not currently assess cancer potency

or perform cancer risk assessments. Minimal risk levels (MRLs) for noncancer end points (if derived) and the end points from which they were derived are indicated and discussed.

Limitations to existing scientific literature that prevent a satisfactory evaluation of the relevance to public health are identified in the Data Needs section.

Interpretation of Minimal Risk Levels

Where sufficient toxicologic information is available, minimal risk levels (MRLs) for inhalation and oral routes of entry at each duration of exposure (acute, intermediate, and chronic) are provided. Though no new MRLs are derived for TPH, all available MRLs for TPH components and petroleum products are reviewed in Chapter 6 and presented in Appendix A. These MRLs are not meant to support regulatory action; but to acquaint health professionals with exposure levels at which adverse health effects are not expected to occur in humans. They should help physicians and public health officials determine the safety of a community living near a chemical emission, given the concentration of a contaminant in air or the estimated daily dose in water. MRLs are based largely on toxicological studies in animals and on reports of human occupational exposure.

MRL users should be familiar with the toxicologic information on which the number is based. In particular, the user should review the profile of the specific substance of concern (see Appendix A). Section 6.7, "Relevance to Public Health," contains basic information known about the substance. Other sections such as 6.9, "Interactions with Other Substances," and 6.10, "Populations that are Unusually Susceptible" provide important supplemental information.

MRL users should also understand the MRL derivation methodology. MRLs are derived using a modified version of the risk assessment methodology the Environmental Protection Agency (EPA) provides (Barnes and Dourson 1988) to determine reference doses for lifetime exposure (RfDs).

To derive an MRL, ATSDR generally selects the most sensitive end point which, in its best judgement, represents the most sensitive human health effect for a given exposure route and duration. ATSDR cannot make this judgement or derive an MRL unless information (quantitative or qualitative) is available for all potential systemic, neurological, and developmental effects. If this information and reliable quantitative data on the chosen end point are available, ATSDR derives an MRL using the most sensitive species (when information from multiple species is available) with the highest NOAEL that does not exceed any adverse effect levels. When a NOAEL is not available, a lowest-observed-adverse-effect level (LOAEL) can be used to derive an MRL, and an uncertainty factor (UP) of 10 must be employed. Additional uncertainty factors of 10 must be used both for human variability to protect sensitive subpopulations (people who are most susceptible to the health effects caused by the substance) and for interspecies variability (extrapolation from animals to humans). In deriving an MRL, these individual uncertainty factors are multiplied together. The product is then divided into the inhalation concentration or oral dosage selected from the study. Uncertainty factors used in developing a substance-specific MRL are provided in the footnotes of the LSE Tables in the profiles listed in Appendix A.

The section covers end points in the same order they appear within the Discussion of Health Effects by Route of Exposure section, by route (inhalation, oral, dermal) and within route by effect. Human data are presented first, then animal data. Both are organized by duration (acute, intermediate, chronic). *In vitro* data and data from parenteral routes (intramuscular, intravenous, subcutaneous, etc.) are also considered in this section. If data are located in the scientific literature, a table of genotoxicity information is included.

APPENDIX C

ACRONYMS, ABBREVIATIONS, AND SYMBOLS

ACGIH	American Conference of Governmental Industrial Hygienists
ADME	Absorption, Distribution, Metabolism, and Excretion
atm	atmosphere
ASTM	American Society for Testing and Materials
ATSDR	Agency for Toxic Substances and Disease Registry
BCF	bioconcentration factor
BSC	Board of Scientific Counselors
BTEX	benzene, toluene, ethylbenzene, xylene
C	Centigrade
CDC	Centers for Disease Control and Prevention
CEL	Cancer Effect Level
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CFR	Code of Federal Regulations
CLP	Contract Laboratory Program
cm	centimeter
CNS	central nervous system
d	day
DHEW	Department of Health, Education, and Welfare
DHHS	Department of Health and Human Services
DNAPL	denser nonaqueous phase liquids
DOL	Department of Labor
EC	equivalent carbon number
ECG	electrocardiogram
EEG	electroencephalogram
EPA	Environmental Protection Agency
EKG	see ECG
DRO	diesel range organics
F	Fahrenheit
F ₁	first filial generation
FAO	Food and Agricultural Organization of the United Nations
FEMA	Federal Emergency Management Agency
FID	flame ionization detection
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
fpm	feet per minute
ft	foot
FR	<i>Federal Register</i>
g	gram
GC	gas chromatography
GC/MS	gas chromatography/mass spectrometry
gen	generation
GRO	gasolines range organics
HEC	human equivalent concentration
HPLC	high-performance liquid chromatography
hr	hour
HSSM	hydrocarbon spill screening model
IDLH	Immediately Dangerous to Life and Health
IARC	International Agency for Research on Cancer

APPENDIX C

IOC	index of concern
ILO	International Labor Organization
in	inch
K _d	adsorption ratio
kg	kilogram
kgg	metric ton
K _{oc}	organic carbon partition coefficient
K _{ow}	octanol-water partition coefficient
L	liter
LC	liquid chromatography
LC _{Lo}	lethal concentration, low
LC ₅₀	lethal concentration, 50% kill
LD _{Lo}	lethal dose, low
LD ₅₀	lethal dose, 50% kill
LNAPL	lighter nonaqueous phase liquids
LOAEL	lowest-observed-adverse-effect level
LSE	Levels of Significant Exposure
LUST	leaking underground storage tanks
m	meter
MADEP	Massachusetts Department of Environmental Protection
MARPOL	International Convention for the Prevention of Pollution Ships (marine pollution)
mg	milligram
min	minute
mL	milliliter
mm	millimeter
mmHg	millimeters of mercury
MTBE	methyl- <i>tert</i> -butyl ether
mmol	millimole
mo	month
mppcf	millions of particles per cubic foot
MRL	Minimal Risk Level
MS	mass spectrometry
NAPL	non-aqueous phase liquids
NIEHS	National Institute of Environmental Health Sciences
NIOSH	National Institute for Occupational Safety and Health
NIOSHTIC	NIOSH's Computerized Information Retrieval System
ng	nanogram
nm	nanometer
NHANES	National Health and Nutrition Examination Survey
nmol	nanomole
NOAEL	no-observed-adverse-effect level
NOES	National Occupational Exposure Survey
NOHS	National Occupational Hazard Survey
NPDES	National Pollutant Discharge Elimination System
NPL	National Priorities List
NRC	National Research Council
NTIS	National Technical Information Service
NTP	National Toxicology Program
OSHA	Occupational Safety and Health Administration
PAHs	polyaromatic hydrocarbons
PCBs	polychlorinated biphenyls

APPENDIX C

PEL	permissible exposure limit
pg	picogram
PID	photo ionization detector
pmol	picomole
PHS	Public Health Service
PMR	proportionate mortality ratio
ppb	parts per billion
ppm	parts per million
ppt	parts per trillion
RBCA	Risk-Based Corrective Action
RBSL	risk-based screening level
RCRA	Resource Conservation and Recovery Act
REL	recommended exposure limit
RfC	Reference Concentration
RfD	Reference Dose
RP	relative potency
RQ	reportable quantity
RTECS	Registry of Toxic Effects of Chemical Substances
sec	second
SCE	sister chromatid exchange
SFE	supercritical fluid extraction
SIC	Standard Industrial Classification
SMR	standard mortality ratio
spcc	spill prevention, control and countermeasure
SPE	solid phase extraction
SSTL	site-specific target level
STEL	short term exposure limit
STORET	STORAGE and RETRIEVAL
TOG	total recoverable oil and grease
TPH	total petroleum hydrocarbons
TPHCWG	Total Petroleum Hydrocarbons Criteria Working Group
TRPH	total recoverable petroleum hydrocarbons
TSCA	Toxic Substances Control Act (TSCA)
TLV	threshold limit value
TSCA	Toxic Substances Control Act
TSDF	treatment, storage and disposal facilities, hazardous wastes
TRI	Toxics Release Inventory
TWA	time-weighted average
U.S.	United States
UF	uncertainty factor
UST	underground storage tank
yr	year
WHO	World Health Organization
wk	week
WOE	weight-of-evidence, classification of carcinogenicity

APPENDIX C

>	greater than
≥	greater than or equal to
=	equal to
<	less than
≤	less than or equal to
%	percent
α	alpha
β	beta
δ	delta
γ	gamma
μm	micrometer
μg	microgram

APPENDIX D

PETROLEUM PRODUCT COMPOSITION

Petroleum products can be made up of hundreds of individual petroleum hydrocarbons. TPH is a value that represents the amount of petroleum hydrocarbons in a given sample, as previously presented in Section 2.1. There are far more than 250 individual chemicals that are known as petroleum hydrocarbons and there is an inherent complexity involved in chemically and physically describing and categorizing these components.

This Appendix contains a list of the more prominent individual chemicals that are likely to be associated with TPH. Table D-1 sorts the petroleum hydrocarbons into groups based upon basic chemical structure. An "ATSDR Fraction" column identifies which one of six particular fractions individual chemicals have been assigned to for health effects purposes, as described in Section 6.1.3 and shown below.

Aliph1 = Aliphatics EC₅-EC₈

Aliph2 = Aliphatics EC_{>8}-EC₁₆

Aliph3 = Aliphatics EC_{>16}-EC₃₅

Arom1 = Aromatics EC₅-EC₉

Arom2 = Aromatics EC_{>9}-EC₁₆

Arom3 = Aromatics EC_{>16}-EC₃₅

APPENDIX D

Table D-1. Petroleum Product Composition

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
Straight Chain Alkanes						
Propane	3	3		0.01–0.14	Gasoline	LUFT 1988
n-Butane	4	4		3.93–4.70	Gasoline	LUFT 1988
				0.12	JP-4	API 1993
n-Pentane	5	5	<i>Aliph1</i>	5.75–10.92	Gasoline	LUFT 1988
				1.06	JP-4	API 1993
n-Hexane	6	6	<i>Aliph1</i>	0.24–3.50	Gasoline	LUFT 1988
				0.7–1.8	Crude Oil	API 1993
				2.21	JP-4	API 1993
n-Heptane	7	7	<i>Aliph1</i>	0.31–1.96	Gasoline	LUFT 1988
				0.8–2.3	Crude Oil	API 1993
				3.67	JP-4	API 1993
				0.03	JP-8	API 1993
				0.1	Kerosene	API 1993
n-Octane	8	8	<i>Aliph1</i>	0.36–1.43	Gasoline	LUFT 1988
				0.9–1.9	Crude Oil	API 1993
				3.8	JP-4	API 1993
				0.12	JP-5	API 1993
				0.9	JP-8	API 1993
				0.2–0.3	Kerosene	API 1993
				0.1	Diesel	BP 1996
				0.1	Fuel Oil #2	BP 1996

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
n-Nonane	9	9	<i>Aliph2</i>	0.07–0.83	Gasoline	LUFT 1988
				0.6–1.9	Crude Oil	API 1993
				2.25	JP-4	API 1993
				0.38	JP-5	API 1993
				0.31	JP-8	API 1993
				0.4–0.8	Kerosene	API 1993
				0.19–0.49	Diesel	BP 1996
				0.20–0.30	Fuel Oil #2	BP 1996
n-Decane	10	10	<i>Aliph2</i>	0.04–0.50	Gasoline	LUFT 1988
				1.8	Crude Oil	API 1993
				2.16	JP-4	API 1993
				1.79	JP-5	API 1993
				1.31	JP-8	API 1993
				1.5–1.7	Kerosene	API 1993
				0.28–1.2	Diesel	BP 1996
				0.5	Fuel Oil #2	BP 1996
n-Undecane	11	11	<i>Aliph2</i>	0.05–0.22	Gasoline	LUFT 1988
				1.7	Crude Oil	API 1993
				2.32	JP-4	API 1993
				3.95	JP-5	API 1993
				4.13	JP-8	API 1993
				3.5–6.1	Kerosene	API 1993
				0.57–2.3	Diesel	BP 1996
				0.80–0.90	Fuel Oil #2	BP 1996

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
n-Dodecane	12	12	<i>Aliph2</i>	0.04–0.09	Gasoline	LUFT 1988
				1.7	Crude Oil	API 1993
				2	JP-4	API 1993
				3.94	JP-5	API 1993
				4.72	JP-8	API 1993
				2.8–5.7	Kerosene	API 1993
				1.0–2.5	Diesel	BP 1996
				0.84–1.20	Fuel Oil #2	BP 1996
n-Tridecane	13	13	<i>Aliph2</i>	1.52	JP-4	API 1993
				3.45	JP-5	API 1993
				4.43	JP-8	API 1993
				3.1–5.2	Kerosene	API 1993
				1.5–2.8	Diesel	BP 1996
				0.96–2.00	Fuel Oil #2	BP 1996
n-Tetradecane	14	14	<i>Aliph2</i>	0.73	JP-4	API 1993
				2.72	JP-5	API 1993
				2.99	JP-8	API 1993
				2.3–4.7	Kerosene	API 1993
				0.61–2.7	Diesel	BP 1996
				1.03–2.50	Fuel Oil #2	BP 1996
				n-Pentadecane	15	15
1.61	JP-8	API 1993				
0.6–2.3	Kerosene	API 1993				
1.9–3.1	Diesel	BP 1996				
1.13–3.20	Fuel Oil #2	BP 1996				

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
n-Hexadecane	16	16	<i>Aliph2</i>	1.07	JP-5	API 1993
				0.45	JP-8	API 1993
				0.1–0.7	Kerosene	API 1993
				1.5–2.8	Diesel	BP 1996
				1.05–3.30	Fuel Oil #2	BP 1996
n-Heptadecane	17	17	<i>Aliph3</i>	0.12	JP-5	API 1993
				0.08	JP-8	API 1993
				0.4	Kerosene	API 1993
				1.4–2.9	Diesel	BP 1996
				0.65–3.60	Fuel Oil #2	BP 1996
n-Octadecane	18	18	<i>Aliph3</i>	0.02	JP-8	API 1993
				0.3	Kerosene	API 1993
				1.2–2.0	Diesel	BP 1996
				0.55–2.50	Fuel Oil #2	BP 1996
n-Nonadecane	19	19	<i>Aliph3</i>	0.2	Kerosene	API 1993
				0.7–1.5	Diesel	BP 1996
				0.33–1.30	Fuel Oil #2	BP 1996
n-Eicosane	20	20	<i>Aliph3</i>	0.1	Kerosene	API 1993
				0.4–1.0	Diesel	BP 1996
				0.18–0.60	Fuel Oil #2	BP 1996
n-Heneicosane	21	21	<i>Aliph3</i>	0.1	Kerosene	API 1993
				0.26–0.83	Diesel	BP 1996
				0.09–0.40	Fuel Oil #2	BP 1996
n-Docosane	22	22	<i>Aliph3</i>	0.14–0.44	Diesel	BP 1996

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
				0.1	Fuel Oil #2	BP 1996
n-Tetracosane	24	24	<i>Aliph3</i>	0.35	Diesel	BP 1996
n-Hexacosane	26	26	<i>Aliph3</i>			
Branched Chain Alkanes						
Isobutane	4	3.67		0.12–0.37	Gasoline	LUFT 1988
				0.66	JP-4	API 1993
2,2-Dimethylbutane	6	5.37	<i>Aliph1</i>	0.17–0.84	Gasoline	LUFT 1988
				0.04	Crude Oil	API 1993
				0.1	JP-4	API 1993
2,3-Dimethylbutane	6	5.68	<i>Aliph1</i>	0.59–1.55	Gasoline	LUFT 1988
				0.04–0.14	Crude Oil	API 1993
2,2,3-Trimethylbutane	7	6.36	<i>Aliph1</i>	0.01–0.04	Gasoline	LUFT 1988
2,2,3,3-Tetramethylbutane	8	7.3	<i>Aliph1</i>	0.24	JP-4	API 1993
Neopentane	5	4.32		0.02–0.05	Gasoline	LUFT 1988
Isopentane	5	4.75		6.07–10.17	Gasoline	LUFT 1988
2-Methylpentane	6	5.72	<i>Aliph1</i>	2.91–3.85	Gasoline	LUFT 1988
				0.3–0.4	Crude Oil	API 1993
				1.28	JP-4	API 1993
3-Methylpentane	6	5.85	<i>Aliph1</i>	2.4 (vol)	Gasoline	LUFT 1988
				0.3–0.4	Crude Oil	API 1993
				0.89	JP-4	API 1993
3-Ethylpentane	7		<i>Aliph1</i>	0.05	Crude Oil	API 1993
2,2-Dimethylpentane	7	6.25	<i>Aliph1</i>	0.25	JP-4	API 1993
2,4-Dimethylpentane	7	6.31	<i>Aliph1</i>	0.23–1.71	Gasoline	LUFT 1988
				0.05	Crude Oil	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
2,3-Dimethylpentane	7	6.69	<i>Aliph1</i>	0.32–4.17	Gasoline	LUFT 1988
				0.1–0.6	Crude Oil	API 1993
3,3-Dimethylpentane	7	6.55	<i>Aliph1</i>	0.02–0.03	Gasoline	LUFT 1988
2,2,3-Trimethylpentane	8	7.37	<i>Aliph1</i>	0.09–0.23	Gasoline	LUFT 1988
2,2,4-Trimethylpentane	8	6.89	<i>Aliph1</i>	0.32–4.58	Gasoline	LUFT 1988
				0.004	Crude Oil	API 1993
2,3,3-Trimethylpentane	8	7.58	<i>Aliph1</i>	0.05–2.28	Gasoline	LUFT 1988
				0.006	Crude Oil	API 1993
2,3,4-Trimethylpentane	8	7.55	<i>Aliph1</i>	0.11–2.80	Gasoline	LUFT 1988
				0.005	Crude Oil	API 1993
2-Methyl-3-ethylpentane	8	7.66	<i>Aliph1</i>	0.04	Crude Oil	API 1993
2,4-Dimethyl-3-ethylpentane	9		<i>Aliph2</i>	0.03–0.07	Gasoline	LUFT 1988
2-Methylhexane	7	6	<i>Aliph1</i>	68 0.36–1.48	Gasoline	LUFT 1988
				0.7	Crude Oil	API 1993
				2.35	JP-4	API 1993
3-Methylhexane	7	6.76	<i>Aliph1</i>	0.30–1.77	Gasoline	LUFT 1988
				0.19–0.5	Crude Oil	API 1993
				1.97	JP-4	API 1993
2,2-Dimethylhexane	8	7.25	<i>Aliph1</i>	0.01–0.1	Crude Oil	API 1993
				0.71	JP-4	API 1993
2,3-Dimethylhexane	8	7.65	<i>Aliph1</i>	0.06–0.16	Crude Oil	API 1993
2,4-Dimethylhexane	8	7.38	<i>Aliph1</i>	0.34–0.82	Gasoline	LUFT 1988
				0.06	Crude Oil	API 1993
				0.58	JP-4	API 1993
2,5-Dimethylhexane	8	7.36	<i>Aliph1</i>	0.24–0.52	Gasoline	LUFT 1988

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
				0.06	Crude Oil	API 1993
				0.37	JP-4	API 1993
3,3-Dimethylhexane	8	7.45	<i>Aliph1</i>	0.03	Crude Oil	API 1993
				0.26	JP-4	API 1993
3,4-Dimethylhexane	8	7.74	<i>Aliph1</i>	0.16–0.37	Gasoline	LUFT 1988
3-Ethylhexane	8	7.79	<i>Aliph1</i>	0.01	Gasoline	LUFT 1988
2-Methyl-3-ethylhexane	9			0.04–0.13	Gasoline	LUFT 1988
2,2,4-Trimethylhexane	9	7.93	<i>Aliph1</i>	0.11–0.18	Gasoline	LUFT 1988
2,2,5-Trimethylhexane	9	7.87	<i>Aliph1</i>	0.17–5.89	Gasoline	LUFT 1988
2,3,3-Trimethylhexane	9			0.05–0.12	Gasoline	LUFT 1988
2,3,5-Trimethylhexane	9	8.24	<i>Aliph2</i>	0.05–1.09	Gasoline	LUFT 1988
2,4,4-Trimethylhexane	9	8.07		0.02–0.16	Gasoline	LUFT 1988
2-Methylheptane	8	7.71	<i>Aliph1</i>	0.48–1.05	Gasoline	LUFT 1988
				2.7	JP-4	API 1993
3-Methylheptane	8	7.78	<i>Aliph1</i>	0.63–1.54	Gasoline	LUFT 1988
				3.04	JP-4	API 1993
4-Methylheptane	8	7.72	<i>Aliph1</i>	0.22–0.52	Gasoline	LUFT 1988
				0.92	JP-4	API 1993
2,2-Dimethylheptane	9	8.28	<i>Aliph2</i>	0.01–0.08	Gasoline	LUFT 1988
2,3-Dimethylheptane	9	8.64	<i>Aliph2</i>	0.13–0.51	Gasoline	LUFT 1988
				0.05	Crude Oil	API 1993
2,4-Dimethylheptane	9	8.34	<i>Aliph2</i>	0.43	JP-4	API 1993
2,5-Dimethylheptane	9	8.47	<i>Aliph2</i>	0.52	JP-4	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
2,6-Dimethylheptane	9	8.47	<i>Aliph2</i>	0.07–0.23	Gasoline	LUFT 1988
				0.05–0.25	Crude Oil	API 1993
3,3-Dimethylheptane	9	8.42		0.01–0.08	Gasoline	LUFT 1988
3,4-Dimethylheptane	9	8.62	<i>Aliph2</i>	0.07–0.33	Gasoline	LUFT 1988
2,2,4-Trimethylheptane	10		<i>Aliph2</i>	0.12–1.70	Gasoline	LUFT 1988
2,4,6-Trimethylheptane	10		<i>Aliph2</i>	0.07	JP-5	API 1993
3,3,5-Trimethylheptane	10		<i>Aliph2</i>	0.02–0.06	Gasoline	LUFT 1988
3-Ethylheptane	9	8.77	<i>Aliph2</i>	0.02–0.16	Gasoline	LUFT 1988
4-Ethylheptane	9	8.69	<i>Aliph2</i>	0.18	JP-4	API 1993
2-Methyloctane	9		<i>Aliph2</i>	0.14–0.62	Gasoline	LUFT 1988
				0.4	Crude Oil	API 1993
				0.88	JP-4	API 1993
3-Methyloctane	9	8.78	<i>Aliph2</i>	0.34–0.85	Gasoline	LUFT 1988
				0.1–0.4	Crude Oil	API 1993
				0.79	JP-4	API 1993
				0.07	JP-5	API 1993
				0.04	JP-8	API 1993
4-Methyloctane	9	8.71	<i>Aliph2</i>	0.11–0.55	Gasoline	LUFT 1988
				0.1	Crude Oil	API 1993
				0.86	JP-4	API 1993
2,6-Dimethyloctane	10	9.32	<i>Aliph2</i>	0.06–0.12	Gasoline	LUFT 1988
2-Methylnonane	10	9.72	<i>Aliph2</i>	0.06–0.41	Gasoline	LUFT 1988
3-Methylnonane	10	9.78	<i>Aliph2</i>	0.06–0.32	Gasoline	LUFT 1988
4-Methylnonane	10		<i>Aliph2</i>	0.04–0.26	Gasoline	LUFT 1988
4-Methyldecane	11		<i>Aliph2</i>	0.78	JP-5	API 1993
2-Methyldecane	11		<i>Aliph2</i>	0.61	JP-5	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
				0.41	JP-8	API 1993
2,6-Dimethyldecane	12		<i>Aliph2</i>	0.72	JP-5	API 1993
				0.66	JP-8	API 1993
2-Methylundecane	12		<i>Aliph2</i>	0.64	JP-4	API 1993
				1.39	JP-5	API 1993
				1.16	JP-8	API 1993
3-Methylundecane	12		<i>Aliph2</i>	0.09–0.28	Diesel	BP 1996
2-Methyldodecane	13		<i>Aliph2</i>	0.15–0.52	Diesel	BP 1996
2,6-Dimethylundecane	13		<i>Aliph2</i>	0.71	JP-4	API 1993
				2	JP-5	API 1993
				2.06	JP-8	API 1993
3-Methyltridecane	14		<i>Aliph2</i>	0.13–0.30	Diesel	BP 1996
2-Methyltetradecane	15		<i>Aliph2</i>	0.34–0.63	Diesel	BP 1996
Cycloalkanes						
Cyclopentane	5	5.66	<i>Aliph1</i>	0.19–0.58	Gasoline	LUFT 1988
				0.05	Crude Oil	API 1993
Methylcyclopentane	6	6.27	<i>Aliph1</i>	not quantified	Gasoline	LUFT 1988
				0.3–0.9	Crude Oil	API 1993
				1.16	JP-4	API 1993
1-Methyl-cis-2-ethylcyclopentane	8		<i>Aliph1</i>	0.06–0.11	Gasoline	LUFT 1988
1-Methyl-trans-3-ethylcyclopentane	8		<i>Aliph1</i>	0.06–0.12	Gasoline	LUFT 1988
1,1-Dimethylcyclopentane	7	6.72	<i>Aliph1</i>	0.06–0.2	Crude Oil	API 1993
1-cis-2-Dimethylcyclopentane	7	7.21	<i>Aliph1</i>	0.07–0.13	Gasoline	LUFT 1988
				0.54	JP-4	API 1993
1-Trans-2-dimethylcyclopentane	7	6.87	<i>Aliph1</i>	0.06–0.20	Gasoline	LUFT 1988

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
				0.15–.5	Crude Oil	API 1993
1-cis-3-Dimethylcyclopentane	7	6.82	<i>Aliph1</i>	0.2	Crude Oil	API 1993
				0.34	JP-4	API 1993
1-Trans-3-dimethylcyclopentane	7	6.85	<i>Aliph1</i>	0.2–0.9	Crude Oil	API 1993
				0.36J	P-4	API 1993
1,1,2-Trimethylcyclopentane	8	7.67	<i>Aliph1</i>	0.06–0.1	Gasoline	LUFT 1988
				0.06	Crude Oil	API 1993
1,1,3-Trimethylcyclopentane	8	7.25	<i>Aliph1</i>	0.3	Crude Oil	API 1993
1-Trans-2-cis-3-trimethylcyclopentane	8	7.51	<i>Aliph1</i>	0.01–0.25	Gasoline	LUFT 1988
				0.3–0.4	Crude Oil	API 1993
1-Trans-2-cis-4-trimethylcyclopentane	8			0.03–0.16	Gasoline	LUFT 1988
				0.2	Crude Oil	API 1993
1-Trans-2-trans-4-trimethylcyclopentane	8	7.19	<i>Aliph1</i>			
Ethylcyclopentane	7	7.34	<i>Aliph1</i>	0.14–0.21	Gasoline	LUFT 1988
				0.26	JP-4	API 1993
n-Propylcyclopentane	8	7.1	<i>Aliph1</i>	0.01–0.06	Gasoline	LUFT 1988
Isopropylcyclopentane	8		<i>Aliph1</i>	0.01–0.02	Gasoline	LUFT 1988
1-cis-3-Dimethylcyclohexane	8	7.75	<i>Aliph1</i>	0.42	JP-4	API 1993
1-Trans-2-dimethylcyclohexane	8	7.94	<i>Aliph1</i>	0.3	Crude Oil	API 1993
1-Trans-3-dimethylcyclohexane	8	7.99	<i>Aliph1</i>	0.05–0.12	Gasoline	LUFT 1988
1,4-Dimethylcyclohexane	8					

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
Ethylcyclohexane	8	8.38	<i>Aliph2</i>	0.17–0.42	Gasoline	LUFT 1988
				0.2	Crude Oil	API 1993
Cyclohexane	6	6.59	<i>Aliph1</i>	0.7	Crude Oil	API 1993
				0.08	Gasoline	API 1993
				1.24	JP-4	API 1993
Methylcyclohexane	7	7.22	<i>Aliph1</i>	2.27	JP-4	API 1993
1-Methyl-2-ethyl-cyclohexane	9		<i>Aliph2</i>	0.39	JP-4	API 1993
1-Methyl-3-ethyl-cyclohexane	9		<i>Aliph2</i>	0.17	JP-4	API 1993
1-Methyl-4-ethyl-cyclohexane	9		<i>Aliph2</i>	0.48	JP-5	API 1993
				0.1	JP-8	API 1993
1,3,5-Trimethyl-cyclohexane	9		<i>Aliph2</i>	0.99	JP-4	API 1993
				0.09	JP-5	API 1993
				0.06	JP-8	API 1993
1,1,3-Trimethyl-cyclo-hexane	9	8.45	<i>Aliph2</i>	0.48	JP-4	API 1993
				0.05	JP-5	API 1993
				0.06	JP-8	API 1993
n-Butylcyclohexane	10		<i>Aliph2</i>	0.7	JP-4	API 1993
				0.9	JP-5	API 1993
				0.74	JP-8	API 1993
n-Propylcyclohexane	9		<i>Aliph2</i>	0.14	JP-8	API 1993
Hexylcyclohexane	12		<i>Aliph2</i>	0.93	JP-8	API 1993
Heptylcyclohexane	13		<i>Aliph2</i>	0.99	JP-5	API 1993
				1	JP-8	API 1993
Pentylcyclopentane	10	10.4	<i>Aliph2</i>			
1-Trans-2-trans-4-tri-methylcyclo-hexane	9		<i>Aliph2</i>	0.2	Crude Oil	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
Straight Chained Alkenes						
Propylene	3					
cis-2-Butene	4	4.25		0.13–0.17	Gasoline	LUFT 1988
trans-2-Butene	4	4.1		0.16–0.20	Gasoline	LUFT 1988
Pentene-1	5	4.89		0.33–0.45	Gasoline	LUFT 1988
1-Pentyne	5	5.13	<i>Aliph1</i>			
cis-2-Pentene	5	5.16	<i>Aliph1</i>	0.43–0.67	Gasoline	LUFT 1988
Trans-2-pentene	5	5.08	<i>Aliph1</i>	0.52–0.90	Gasoline	LUFT 1988
1-Hexene	6	5.9	<i>Aliph1</i>			
1-Hexyne	6	6.09	<i>Aliph1</i>			
cis-2-Hexene	6	6.14	<i>Aliph1</i>	0.15–0.24	Gasoline	LUFT 1988
Trans-2-hexene	6	6.05	<i>Aliph1</i>	0.18–0.36	Gasoline	LUFT 1988
cis-3-Hexene	6	6.03	<i>Aliph1</i>	0.11–0.13	Gasoline	LUFT 1988
Trans-3-hexene	6	6.02	<i>Aliph1</i>	0.12–0.15	Gasoline	LUFT 1988
cis-3-Heptene	7	7.01	<i>Aliph1</i>	0.14–0.17	Gasoline	LUFT 1988
Trans-2-heptene	7	7.05	<i>Aliph1</i>	0.06–0.10	Gasoline	LUFT 1988
1-Octene	8	7.89	<i>Aliph1</i>			
1-Nonene	9	8.69	<i>Aliph2</i>			
1-Decene	10	9.91	<i>Aliph2</i>			
Tridecene	13		<i>Aliph2</i>	0.45	JP-5	API 1993
				0.73	JP-8	API 1993
Branched Chain Alkenes						
2-Methyl-1-butene	5	4.96		0.22–0.66	Gasoline	LUFT 1988
3-Methyl-1-butene	5	4.57		0.08–0.12	Gasoline	LUFT 1988
2-Methyl-2-butene	5	5.21	<i>Aliph1</i>	0.96–1.28	Gasoline	LUFT 1988
2,3-Dimethyl-1-butene	6	5.7	<i>Aliph1</i>	0.08–0.10	Gasoline	LUFT 1988
2-Methyl-1-pentene	6	5.89	<i>Aliph1</i>	0.20–0.22	Gasoline	LUFT 1988

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
2,3-Dimethyl-1-pentene	7		<i>Aliph1</i>	0.01–0.02	Gasoline	LUFT 1988
2,4-Dimethyl-1-pentene	7	6.48	<i>Aliph1</i>	0.02–0.03	Gasoline	LUFT 1988
4,4-Dimethyl-1-pentene	7		<i>Aliph1</i>	0.60 (vol)	Gasoline	LUFT 1988
2-Methyl-2-pentene	6	6.07	<i>Aliph1</i>	0.27–0.32	Gasoline	LUFT 1988
3-Methyl-cis-2-pentene	6	6.11	<i>Aliph1</i>	0.35–0.45	Gasoline	LUFT 1988
3-Methyl-trans-2-pentene	6	6.22	<i>Aliph1</i>	0.32–0.44	Gasoline	LUFT 1988
4-Methyl-cis-2-pentene	6	5.69	<i>Aliph1</i>	0.04–0.05	Gasoline	LUFT 1988
4-Methyl-trans-2-pentene	6	5.73	<i>Aliph1</i>	0.08–0.30	Gasoline	LUFT 1988
4,4-Dimethyl-cis-2-pentene	7	6.47	<i>Aliph1</i>	0.02	Gasoline	LUFT 1988
4,4-Dimethyl-trans-2-pentene	7	6.23	<i>Aliph1</i>	Not quantified	Gasoline	LUFT 1988
3-Ethyl-2-pentene	7	7.07	<i>Aliph1</i>	0.03–0.04	Gasoline	LUFT 1988
Cycloalkenes						
Cyclopentene	5	5.55	<i>Aliph1</i>	0.12–0.18	Gasoline	LUFT 1988
3-Methylcyclopentene	6	6.1	<i>Aliph1</i>	0.03–0.08	Gasoline	LUFT 1988
Cyclohexene	6	6.74	<i>Aliph1</i>	0.03	Gasoline	LUFT 1988
Alkyl Benzenes						
Benzene	6	6.5	<i>Arom1</i>	0.12–3.50	Gasoline	LUFT 1988
				0.04–0.4	Crude Oil	API 1993
				0.5	JP-4	API 1993
				0.003–0.10	Diesel	BP 1996
				<0.125	Fuel Oil #2	BP 1996

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
Toluene	7	7.58	<i>Arom1</i>	2.73–21.80	Gasoline	LUFT 1988
				0.09–2.5	Crude Oil	API 1993
				1.33	JP-4	API 1993
				0.007–0.70	Diesel	BP 1996
				0.025–0.110	Fuel Oil #2	BP 1996
Ethylbenzene	8	8.5	<i>Arom1</i>	0.36–2.86	Gasoline	LUFT 1988
				0.09–0.31	Crude Oil	API 1993
				0.37	JP-4	API 1993
				0.007–0.20	Diesel	BP 1996
				0.028–0.04	Fuel Oil #2	BP 1996
o-Xylene	8	8.81	<i>Arom1</i>	0.68–2.86	Gasoline	LUFT 1988
				0.03–0.68	Crude Oil	API 1993
				1.01	JP-4	API 1993
				0.09	JP-5	API 1993
				0.06	JP-8	API 1993
				0.001–0.085	Diesel	BP 1996
m-Xylene	8	8.6	<i>Arom1</i>	1.77–3.87	Gasoline	LUFT 1988
				0.08–2.0	Crude Oil	API 1993
				0.96	JP-4	API 1993
				0.13	JP-5	API 1993
				0.06	JP-8	API 1993
				0.018–0.512	Diesel	BP 1996
p-Xylene	8	8.61	<i>Arom1</i>	0.77–1.58	Gasoline	LUFT 1988
				0.09–0.68	Crude Oil	API 1993
				0.35	JP-4	API 1993
				0.018–0.512	Diesel	BP 1996
Styrene	9	8.83	<i>Arom1</i>	<.002	Diesel	BP 1996

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
1-Methyl-4-ethylbenzene	9	9.57	<i>Arom2</i>	0.18–1.00	Gasoline	LUFT 1988
				0.03–0.13	Crude Oil	API 1993
				0.43	JP-4	API 1993
1-Methyl-2-ethylbenzene	9	9.71	<i>Arom2</i>	0.19–0.56	Gasoline	LUFT 1988
				0.01–0.09	Crude Oil	API 1993
				0.23	JP-4	API 1993
1-Methyl-3-ethylbenzene	9	9.55	<i>Arom2</i>	0.31–2.86	Gasoline	LUFT 1988
				0.04–0.4	Crude Oil	API 1993
				0.49	JP-4	API 1993
1-Methyl-2-n-propylbenzene	10		<i>Arom2</i>	0.01–0.17	Gasoline	LUFT 1988
1-Methyl-3-n-propylbenzene	10		<i>Arom2</i>	0.08–0.56	Gasoline	LUFT 1988
1-Methyl-2-isopropylbenzene	10		<i>Arom2</i>	0.01–0.12	Gasoline	LUFT 1988
				0.29	JP-4	API 1993
				0.56	JP-8	API 1993
1-Methyl-3-isopropylbenzene	10		<i>Arom2</i>	10.09		
1-Methyl-4-isopropylbenzene	10	10.13	<i>Arom2</i>	0.003–0.026	Diesel	BP 1996
1-Methyl-3-t-butylbenzene	11		<i>Arom2</i>	0.03–0.11	Gasoline	LUFT 1988
1-Methyl-4-t-butylbenzene	11	10.92	<i>Arom2</i>	0.04–0.13	Gasoline	LUFT 1988
1,2-Dimethyl-3-ethylbenzene	10	10.93	<i>Arom2</i>	0.02–0.19	Gasoline	LUFT 1988
1,2-Dimethyl-4-ethylbenzene	10	10.75	<i>Arom2</i>	0.50–0.73	Gasoline	LUFT 1988
				0.77	JP-4	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
1,3-Dimethyl-2-ethyl-benzene	10	10.81	<i>Arom2</i>	0.21–0.59	Gasoline	LUFT 1988
1,3-Dimethyl-4-ethylbenzene	10	10.75	<i>Arom2</i>	0.03–0.44	Gasoline	LUFT 1988
1,3-Dimethyl-5-ethylbenzene	10	10.51	<i>Arom2</i>	0.11–0.42	Gasoline	LUFT 1988
				0.61	JP-4	API 1993
				0.62	JP-8	API 1993
1,3-Dimethyl-5-t-butylbenzene	12		<i>Arom2</i>	0.02–0.16	Gasoline	LUFT 1988
1,4-Dimethyl-2-ethylbenzene	10	10.68	<i>Arom2</i>	0.05–0.36	Gasoline	LUFT 1988
				0.7	JP-4	API 1993
1,2,3-Trimethylbenzene	9	10.06	<i>Arom2</i>	0.21–0.48	Gasoline	LUFT 1988
				0.1	Crude Oil	API 1993
1,2,4-Trimethylbenzene	9	9.84	<i>Arom2</i>	0.66–3.30	Gasoline	LUFT 1988
				0.13–0.69	Crude Oil	API 1993
				1.01	JP-4	API 1993
				0.37	JP-5	API 1993
				0.27	JP-8	API 1993
1,3,5-Trimethylbenzene	9	9.62	<i>Arom2</i>	0.13–1.15	Gasoline	LUFT 1988
				0.05–0.18	Crude Oil	API 1993
				0.42	JP-4	API 1993
				0.09–0.24	Diesel	BP 1996
1,2,3,4-Tetramethylbenzene	10	11.57	<i>Arom2</i>	0.02–0.19	Gasoline	LUFT 1988
				0.2	Crude Oil	API 1993
1,2,3,5-Tetramethylbenzene	10	11.09	<i>Arom2</i>	0.14–1.06	Gasoline	LUFT 1988

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
1,2,4,5-Tetramethylbenzene	10	11.05	<i>Arom2</i>	0.05–0.67	Gasoline	LUFT 1988
1,2-Diethylbenzene	10	10.52	<i>Arom2</i>	0.57	Gasoline	LUFT 1988
1,3-Diethylbenzene	10	10.4	<i>Arom2</i>	0.05–0.38	Gasoline	LUFT 1988
				0.46	JP-4	API 1993
				0.61	JP-5	API 1993
1,4-Diethylbenzene	10	10.46	<i>Arom2</i>	0.77	JP-5	API 1993
1,2,4-Triethylbenzene	12	12.29	<i>Arom2</i>	0.72	JP-5	API 1993
				0.99	JP-8	API 1993
1,3,5-Triethylbenzene	12	12.1	<i>Arom2</i>	0.6	JP-8	API 1993
n-Propylbenzene	9	9.47	<i>Arom2</i>	0.08–0.72	Gasoline	LUFT 1988
				0.71	JP-4	API 1993
				0.03–0.048	Diesel	BP 1996
Isopropylbenzene	9	9.13	<i>Arom2</i>	<10.01–0.23	Gasoline	LUFT 1988
				0.3	JP-4	API 1993
				<0.01	Diesel	BP 1996
n-Butylbenzene	10	10.5	<i>Arom2</i>	0.04–0.44	Gasoline	LUFT 1988
				0.031–0.046	Diesel	BP 1996
Isobutylbenzene	10	9.96	<i>Arom2</i>	0.01–0.08	Gasoline	LUFT 1988
sec-Butylbenzene	10	9.98	<i>Arom2</i>	0.01–0.13	Gasoline	LUFT 1988
t-Butylbenzene	10	9.84	<i>Arom2</i>	0.12	Gasoline	LUFT 1988
1-t-Butyl-3,4,5-trimethylbenzene	13		<i>Arom2</i>	0.24	JP-5	API 1993
n-Pentylbenzene	11	11.49	<i>Arom2</i>	0.01–0.14	Gasoline	LUFT 1988
Isopentylbenzene	11		<i>Arom2</i>	0.07–0.17	Gasoline	LUFT 1988
n-Hexylbenzene	12	12.5	<i>Arom2</i>			
n-Heptylbenzene	13		<i>Arom2</i>	0.27	JP-5	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
				0.25	JP-8	API 1993
n-Octylbenzene	14		<i>Arom2</i>	0.78	JP-5	API 1993
				0.61	JP-8	API 1993
Biphenyl	12	14.26	<i>Arom2</i>	0.006–0.04	Crude Oil	API 1993
				0.7	JP-5	API 1993
				0.63	JP-8	API 1993
				0.01–0.12	Diesel	BP 1996
				0.006–0.009	Fuel Oil #2	BP 1996
4-Methylbiphenyl	13	14.92	<i>Arom2</i>			
4,4'-Dimethylbiphenyl	14	16.55	<i>Arom3</i>			
Phenylcyclohexane	12		<i>Arom2</i>	0.82	JP-5	API 1993
				0.87	JP-8	API 1993
Naphtheno-Benzenes						
Acenaphthene	12	15.5	<i>Arom2</i>	0.013–0.022	Fuel Oil #2	BP 1996
Acenaphthylene	12	15.06	<i>Arom2</i>	0.006	Fuel Oil #2	BP 1996
Indan	9	10.27	<i>Arom2</i>	0.25–0.34	Gasoline	LUFT 1988
				0.07	Crude Oil	API 1993
1-Methylindan	10		<i>Arom2</i>	0.04–0.17	Gasoline	LUFT 1988
2-Methylindan	10	11.39	<i>Arom2</i>	0.02–0.10	Gasoline	LUFT 1988
4-Methylindan	10	11.33	<i>Arom2</i>	0.01–0.16	Gasoline	LUFT 1988
5-Methylindan	10	11.28	<i>Arom2</i>	0.09–0.30	Gasoline	LUFT 1988
Tetralin (tetrahydronaphthalene)	10	11.7	<i>Arom2</i>	0.01–0.14	Gasoline	LUFT 1988
				0.03	Crude Oil	API 1993
5-Methyl-tetrahydronaphthalene	11		<i>Arom2</i>	0.08	Crude Oil	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
6-Methylthiohydronaphthalene	11		<i>Arom2</i>	0.09	Crude Oil	API 1993
Fluorene	13	16.55	<i>Arom3</i>	0.003–0.06	Crude Oil	API 1993
				0.034–0.15	Diesel	BP 1996
				0.004–0.045	Fuel Oil #2	BP 1996
1-Methylfluorene	14	17.99	<i>Arom3</i>			
Fluoranthene	16	21.85	<i>Arom3</i>	0.0000007–0.02	Diesel	BP 1996
				0.000047–0.00037	Fuel Oil #2	BP 1996
2,3-Benzofluorene	17	23.83	<i>Arom3</i>			
1,2-Benzofluorene	17	24.2	<i>Arom3</i>	<0.0024	Fuel Oil #2	BP 1996
Benzo(a)fluorene	17		<i>Arom3</i>	<0.0006	Fuel Oil #2	BP 1996
Benzo(ghi)fluoranthene	18		<i>Arom3</i>	<0.0024	Fuel Oil #2	BP 1996
Benz(b)fluoranthene	20	30.14	<i>Arom3</i>	0.0000003–0.000194	Diesel	BP 1996
				<0.0024	Fuel Oil #2	BP 1996
Benz(k)fluoranthene	20	30.14	<i>Arom3</i>	0.0000003–0.000195	Diesel	BP 1996
				<0.00006	Fuel Oil #2	BP 1996
Indeno (1,2,3-cd) pyrene	22	35.01	<i>Arom3</i>	0.000001–0.000097	Diesel	BP 1996
				<0.0012	Fuel Oil #2	BP 1996
Alkyl Naphthalenes						
Naphthalene	10	11.69	<i>Arom2</i>	0.09–0.49	Gasoline	LUFT 1988
				0.02–0.09	Crude Oil	API 1993
				0.5	JP-4	API 1993
				0.57	JP-5	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
				1.14	JP-8	API 1993
				0.01–0.80	Diesel	BP 1996
				0.009–0.40	Fuel Oil #2	BP 1996
1-Methyl-naphthalene	11	12.99	<i>Arom2</i>	0.78	JP-4	API 1993
				1.44	JP-5	API 1993
				1.84	JP-8	API 1993
				0.001–0.81	Diesel	BP 1996
				0.29–0.48	Fuel Oil #2	BP 1996
2-Methyl-naphthalene	11	12.84	<i>Arom2</i>	0.56	JP-4	API 1993
				1.38	JP-5	API 1993
				1.46	JP-8	API 1993
				0.001–1.49	Diesel	BP 1996
				0.36 -1.00	Fuel Oil #2	BP 1996
1,3-Dimethyl-naphthalene	12	14.77	<i>Arom2</i>	0.55–1.28	Diesel	BP 1996
1,4-Dimethyl-naphthalene	12	14.6	<i>Arom2</i>	0.110–0.23	Diesel	BP 1996
				0.043–0.045	Fuel Oil #2	BP 1996
1,5-Dimethyl-naphthalene	12	13.87	<i>Arom2</i>	0.16–0.36	Diesel	BP 1996
2,3-Dimethyl-naphthalene	12	15	<i>Arom2</i>	0.46	JP-5	API 1993
				0.36	JP-8	API 1993
2,6-Dimethyl-naphthalene	12	14.6	<i>Arom2</i>	0.25	JP-4	API 1993
				1.12	JP-5	API 1993
				1.34	JP-8	API 1993

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
1-Ethyl-naphthalene	12	14.41	<i>Arom2</i>	0.32	JP-5	API 1993
				0.33	JP-8	API 1993
2-Ethyl-naphthalene	12	13.99	<i>Arom2</i>			
1,4,5-Trimethyl-naphthalene	13	10.6	<i>Arom2</i>			
1-Phenyl-naphthalene	16		<i>Arom3</i>			
Polynuclear Aromatics						
Anthracene	14	19.43	<i>Arom3</i>	0.000003 -0.02	Diesel	BP 1996
				0.00010–0.011	Fuel Oil #2	BP 1996
2-Methyl anthracene	15	20.73	<i>Arom3</i>	0.000015–0.018	Diesel	BP 1996
				0.009–0.017	Fuel Oil #2	BP 1996
9-Methyl anthracene	15	20.45	<i>Arom3</i>			
2-Ethyl anthracene	16		<i>Arom3</i>			
9,10-Dimethyl anthracene	16		<i>Arom3</i>	0.002–0.006	Fuel Oil #2	BP 1996
Phenanthrene	14	19.36	<i>Arom3</i>	0.003–0.05	Crude Oil	API 1993
				0.000027–0.30	Diesel	BP 1996
				0.009 -0.170	Fuel Oil #2	BP 1996
1-Methyl-phenanthrene	15	20.73	<i>Arom3</i>	0.000011–0.024	Diesel	BP 1996
				0.017	Fuel Oil #2	BP 1996
2-Methyl-phenanthrene	15		<i>Arom3</i>	0.014–0.18	Diesel	BP 1996
				0.768	Fuel Oil #2	BP 1996
3-Methyl-phenanthrene	15		<i>Arom3</i>	0.000013–0.011	Diesel	BP 1996
4- & 9-Methyl-phenanthrene	15		<i>Arom3</i>	0.00001–0.034	Diesel	BP 1996

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
Pyrene	16	20.8	<i>Arom3</i>	Not quantified	Gasoline	LUFT 1988
				0.000018–0.015	Diesel	BP 1996
				0.00–0.012	Fuel Oil #2	BP 1996
1-Methylpyrene	17		<i>Arom3</i>	0.0000024–0.00137	Diesel	BP 1996
2-Methylpyrene	17		<i>Arom3</i>	0.0000037–0.00106	Diesel	BP 1996
Benz(a)anthracene	18	26.37	<i>Arom3</i>	Not quantified	Gasoline	LUFT 1988
				0.0000021–0.00067	Diesel	BP 1996
				0.000002–0.00012	Fuel Oil #2	BP 1996
Chrysene	18	27.41	<i>Arom3</i>	0.000045	Diesel	BP 1996
				0.000037–0.00039	Fuel Oil #2	BP 1996
Triphenylene	18	26.61	<i>Arom3</i>	0.00033	Diesel	BP 1996
				0.00002–0.00014	Fuel Oil #2	BP 1996
Cyclopenta(cd)-pyrene	18		<i>Arom3</i>	0.000002–0.0000365	Diesel	BP 1996
1-Methyl-7-isopropyl-phenanthrene	18		<i>Arom3</i>	0.0000015–0.00399	Diesel	BP 1996
3-Methylchrysene	19		<i>Arom3</i>	<0.001	Diesel	BP 1996
5-Methylchrysene	19		<i>Arom3</i>			
6-Methylchrysene	19		<i>Arom3</i>	<0.0005	Diesel	BP 1996
Benzo(a)pyrene	20	31.34	<i>Arom3</i>	0.000019–0.00028	Gasoline	LUFT 1988
				0.000005–0.00084	Diesel	BP 1996
				0.000001–0.000060	Fuel Oil #2	BP 1996
Benz(e)pyrene	20	31.17	<i>Arom3</i>	Not quantified	Gasoline	LUFT 1988

APPENDIX D

Table D-1. Petroleum Product Composition (continued)

Compound	Carbon Number	EC ^a	ATSDR Fraction ^b	Weight Percent	Fuel Type	Reference
				0.0000054– 0.000240	Diesel	BP 1996
				0.0000020– 0.000010	Fuel Oil #2	BP 1996
Benzo(ghi)pyrene	20		<i>Arom3</i>	0.0000010– 0.0000070	Fuel Oil #2	BP 1996
Perylene	20	31.34	<i>Arom3</i>	<0.0001	Diesel	BP 1996
				<0.0024	Fuel Oil #2	BP 1996
3-Methyl-cholanthrene	21		<i>Arom3</i>	<0.00006	Fuel Oil #2	BP 1996
Benzo(b)chrysene	22		<i>Arom3</i>	<0.0036	Fuel Oil #2	BP 1996
Benz(ghi)perylene	22	34.01	<i>Arom3</i>	Not quantified	Gasoline	LUFT 1988
				0.0000009– 0.00004	Diesel	BP 1996
				20.0000057	Fuel Oil #2	BP 1996
Picene	22		<i>Arom3</i>	0.0000004– 0.000083	Diesel	BP 1996
				<0.00012	Fuel Oil #2	BP 1996
1,2,5,6-Dibenz-anthracene	22	33.92	<i>Arom3</i>			
Coronene	24	34.01	<i>Arom3</i>	<0.000024	Fuel Oil #2	BP 1996

^a Effective Carbon Number Index

^b Aliph1 = Aliphatics EC₅-EC₈; Arom1 = Aromatics EC₅-EC₉
 Aliph2 = Aliphatics EC_{>8}-EC₁₆; Arom2 = Aromatics EC_{>9}-EC₁₆
 Aliph3 = Aliphatics EC_{>16}-EC₃₅; Arom3 = Aromatics EC_{>16}-EC₃₅

Source: Total Petroleum Hydrocarbons Criteria Working Group. 1997. Selection of Representative TPH Fractions Based on Fate and Transport Considerations, vol. 3.

APPENDIX E

IDENTITY, COMPONENTS, AND CHEMICAL/PHYSICAL PROPERTIES OF SELECTED PETROLEUM PRODUCTS

TPH is a value that represents the amount of petroleum hydrocarbons in a given sample, as previously presented in Section 2.1. There are far more than 250 individual chemicals that are known as petroleum hydrocarbons. Some of these are listed in Appendix D. More often, many of the petroleum hydrocarbons are known by the names associated with the more common whole petroleum products, such as gasoline, fuel oil, mineral oil, and jet fuels, for example. These whole products are actually mixtures of numerous individual compounds, such as those listed in Appendix D, as well as, sometimes, non-petroleum hydrocarbon additives. Because of the complexity involved in chemically and physically describing and categorizing these whole products this Appendix contains more detailed information about the more prominent products that are likely to be associated with TPH. A list of the information is given below.

- E-1. Automotive Gasoline
 - A. Chemical Identity
 - B. Composition
 - C. Chemical and Physical Properties

- E-2. Stoddard Solvent
 - A. Chemical Identity
 - B. Composition
 - C. Chemical and Physical Properties

- E-3. JP-4
 - A. Chemical Identity
 - B. Composition
 - C. Chemical and Physical Properties

- E-4. Fuel Oil
 - A. Chemical Identity
 - B. Composition
 - C. Chemical and Physical Properties

- E-5. Crankcase Oils, Mineral-based
 - A. Chemical Identity
 - B. Composition
 - C. Chemical and Physical Properties

- E-6. Mineral Oil
 - A. Chemical Identity
 - B. Chemical and Physical Properties

APPENDIX E

Table E-1.a. Chemical Identity of Gasoline^a

Character	Information	Reference
Chemical Name	Gasoline	RTECS 1995
Synonym(s)	Casing head gasoline, natural gasoline petrol, motor fuel, motor spirit	RTECS 1995; ATSDR 1995a
Identification Numbers:		
CAS Registry	8006-61-9	RTECS 1995
NIOSH RTECS	LX3300000	RTECS 1995
EPA Hazardous Waste	No data	
OHM/TADS	7217073	OHM/TADS 1991
DOT/UN/NA/IMCO shipping	UN1203, UN1257	RTECS 1995
HSDB	No data	
NCI	No data	

^a Gasoline is a mixture of C-4 through C-12 hydrocarbons, primarily consisting of 4–8% alkanes, 2–5% alkenes, 25–40% isoalkanes, 3–7% cycloalkanes, 1–4% cycloalkenes, and 20–50% aromatics.

Source: ATSDR (1995a)

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data Systems; RTECS = Registry of Toxic Effects of Chemical Substances

APPENDIX E

Table E-1.b. Major Hydrocarbon Components of Gasoline

Fraction Compound	Gasoline Weight Percent Range	Gasoline Weight Percent Mean
C6 Aromatics		
Benzene	0.12–3.50	2.34
C3–C6 Aliphatic		
Propane	0.01–0.14	0.00666
n-Butane	3.93–4.70	3.57
Isobutane	0.12–0.37	0.316
n-Pentane	5.75–10.92	3.18
n-Hexane	0.24–3.50	2.61
2,2-Dimethylbutane	0.17–0.84	0.304
2,3-Dimethylbutane	0.59–1.55	1.41
Neopentane	0.02–0.05	
Isopentane	6.07–10.17	6.22
2-Methylpentane	2.91–3.85	3.35
3-Methylpentane	2.4 (vol)	2.14
Cyclopentane	0.19–0.58	0.131
Methylcyclopentane	not quantified	2.08
Cyclohexane		0.722
1-Pentene	0.33–0.45	0.222
1-Pentyne		
cis-2-Pentene	0.43–0.67	0.865
1-Hexene		0.22
1-Hexyne		
3-Methyl-1-butene	0.08–0.12	0.417
2-Methyl-1-Pentene	0.20–0.22	0.258
Cyclopentene	0.12–0.18	0.236
Cyclohexene	0.03	

APPENDIX E

Table E-1.b. Major Hydrocarbon Components of Gasoline (continued)

Fraction Compound	Gasoline Weight Percent Range	Gasoline Weight Percent Mean
C7–C8 Aromatics		
Toulene	2.73–21.80	8.21
Ethylbenzene	0.36–2.86	1.9
o-Xylene	0.68–2.86	2.71
m-Xylene	1.77–3.87	3.5
p-Xylene	0.77–1.58	3.5
Styrene		
C7–C8 Aliphatics		
n- Heptane	0.31–1.96	1.14
n-Octane	0.36–1.43	0.426
2,2,3-Trimethylbutane	0.01–0.04	0.025
2,2-Dimethylpentane	0.25	0.0878
2,4-Dimethylpentane	0.23–1.71	0.734
2,3-Dimethylpentane	0.32–4.17	1.54
3,3-Dimethylpentane	0.02–0.03	0.0989
2,2,4-Trimethylpentane	0.32–4.58	1.64
2,3,4-Trimethylpentane	0.11–2.80	0.519
2-Methylhexane	0.36–1.48	1.44
3-Methylhexane	0.30–1.77	1.5
2-Methylheptane	0.48–1.05	0.614
3-Methylheptane	0.63–1.54	0.647
1,1,3-Trimethylcyclo-pentane	0.3	0.0511
1-Trans-2-trans-4-Trimethylcyclopentane		
n-Propylcyclopentane	0.01–0.06	
1-Trans-2-dimethyl-cyclohexane		
1-Trans-4-dimethylcyclohexane		0.142
Methylcyclohexane		0.611

APPENDIX E

Table E-1.b. Major Hydrocarbon Components of Gasoline (continued)

Fraction Compound	Gasoline Weight Percent Range	Gasoline Weight Percent Mean
Trans-2-heptene	0.06–0.10	0.105
1-Octene		0.101
C9–C10 Aromatics		
1-Methyl-4-ethylbenzene	0.18–1.00	0.837
1-Methyl-2-ethylbenzene	0.19–0.56	2.89
1-Methyl-4-isopropylbenzene		
1,2,3-trimethylbenzene	0.21–0.48	0.766
1,2,4-trimethylbenzene	0.66–3.30	3.41
1,3,5-trimethylbenzene	0.13–1.15	1.14
1,2,4,5-tetramethyl-benzene	0.05–0.67	
n-Propylbenzene	0.08–0.72	0.648
Isopropylbenzene	<0.01–0.23	
n-Butylbenzene	0.04–0.44	
Isobutylbenzene	0.01–0.08	
sec-Butylbenzene	0.01–0.13	
t-Butylbenzene	0.12	
Indan	0.25–0.34	
Tetralin (tetrahydronaphthalene)	0.01–0.14	
Naphthalene	0.09–0.49	
C9–C10 Aliphatics		
n-Nonane	0.07–0.83	0.243
n-Decane	0.04–0.50	0.26
2,2,5-Trimethylhexane	0.17–5.89	0.177
4-Methyloctane	0.11–0.55	0.5
1,1,3-Trimethylcyclo-hexane		
Pentylcyclopentane		
1-Nonene		
1-Decene		

APPENDIX E

Table E-1.b. Major Hydrocarbon Components of Gasoline (continued)

Fraction Compound	Gasoline Weight Percent Range	Gasoline Weight Percent Mean
C11–C12 Aromatics		
n-Pentylbenzene	0.01–0.14	
n-Hexylbenzene		
Biphenyl		
Acenaphthene		
Acenaphthylene		
1-Methylnaphthalene		
1,4-Dimethyl-naphthalene		
2,3-Dimethyl-naphthalene		
2,6-Dimethylnaphthalene		
1-Ethylnaphthalene		
2-Ethylnaphthalene		
C11-C12 Aliphatics		
n-Undecane	0.05–0.22	
n-Dodecane	0.04–0.09	
C13-C16 Aromatics		
Fluorene		
Fluoranthene		
1,4,5-Trimethylnaphthalene		
Anthracene		
9-Methyl anthracene		
Phenanthrene		
Pyrene	Not quantified	
C13–C16 Aliphatics		
n-Tetradecane		
n-Hexadecane		
C17–and up Aromatics		
Benz(k)fluoranthene		

APPENDIX E

Table E-1.b. Major Hydrocarbon Components of Gasoline (continued)

Fraction Compound	Gasoline Weight Percent Range	Gasoline Weight Percent Mean
Benz(a)anthracene	Not quantified	
Chrysene		
Triphenylene		
Benzo(a)pyrene	0.19–2.8 mg/kg	
Benz(e)pyrene	Not quantified	
Perylene		
3-Methylcholanthrene		
Benz(ghi)perylene	Not quantified	
1,2,5,6-dibenz anthracene		
C17–and up Aliphatics		
n-Octadecane		
n-Eicosane		

Source: Table taken from EA Engineering 1995, *Total Petroleum Hydrocarbon Criteria, Working Group Project #3, Based on Fate and Transport Considerations*, Prepared for Armstrong Laboratory, Brooks Air Force Base, Occupational Medicine, Brooks Air Force Base, Texas, Prepared by EA Engineering, Science, and Technology, Lafayette, California.

APPENDIX E

Table E-1c. Physical and Chemical Properties of Gasoline

Property	Information	Reference
Molecular weight	108 ^a	ATSDR 1995a
Color	Colorless to pale brown	Sax and Lewis 1989
Physical state	Liquid	Sax and Lewis 1989
Melting point	No data	
Boiling point	Initially, 39 °C After 10% distilled, 60 °C After 50% distilled, 110 °C After 90% distilled, 170 °C Final boiling point, 204 °C	Sax and Lewis 1989
Density	0.7–0.8 g/cm ^{3b}	IARC 1998
Odor	Gasoline	Weiss 1986
Odor threshold	0.025 ppm ^c	Weiss 1986
Solubility		
Water at 20 °C	Insoluble	Sax and Lewis 1989
Organic solvent(s)	Absolute alcohol, ether, chloroform, benzene	Sax and Lewis 1989
Partition coefficients		
Log K _{ow}	2.13–4.87 ^d	U.S. Air Force 1989
Log K _{oc}	1.81–4.56 ^d	U.S. Air Force 1989
Vapor pressure ^e		
at 60 °C	465 mm Hg	ASTM 1989
at 56 °C	518 mm Hg	
at 51 °C	593 mm Hg	
at 47 °C	698 mm Hg	
at 41 °C	773 mm Hg	
Henry's law constant at 20 °C	4.8x10 ⁻⁴ m ³ /mol ^d	U.S. Air Force 1989
Autoignition temperature	280–486 °C	Sax and Lewis 1989; Weiss
Flashpoint	-46 °C	Sax and Lewis 1989
Flammability limits	1.4–7.4%	Weiss 1986
Conversion factors	No data	
Explosive limits	1.3–6.0%	Sax and Lewis 1989

^a Average molecular weight

^b Temperature not specified

^c Not specified whether data for air or water

^d Since data are not available for gasoline, ranges are given indicating different values for the individual components.

^e The American Society for Testing and Materials (ASTM) has established guidelines on compositions of gasoline that will permit satisfactory performance under varying conditions. These guidelines define 5 volatility classes that vary by seasonal climatic changes. The values given for vapor pressure at the given temperatures are based on these volatility classes.

APPENDIX E

Table E-2.a. Chemical Identity of Stoddard Solvent^a

Character	Information	Reference
Chemical Name	Stoddard solvent	ATSDR 1995b
Synonym(s)	Dry cleaning safety solvent, naphtha safety solvent, PD-680, petroleum solvent, spotting naphtha, varnoline, white spirits	ATSDR 1995b; U.S. Air Force 1989
Registered Trade Name(s)	Texsolve S, Varsol 1	ATSDR 1995b
Identification Numbers:		
CAS Registry	8052-41-3	ATSDR 1995b
NIOSH RTECS	WJ8925000	ATSDR 1995b
EPA Hazardous Waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	1268 27	ATSDR 1995b
HSDB	No data	
NCI	No data	

^a Stoddard solvent is a mixture of C-7 through C-12 hydrocarbons primarily containing 30-50% linear and branched alkanes, 30-40% cycloalkanes, and 10-20% aromatic hydrocarbons.

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute
 NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data Systems; RTECS = Registry of Toxic Effects of Chemical Substances

Table E-2.b. Possible Formulations of Stoddard Solvent (Percent)

Hydrocarbons	Stoddard solvent ^a (regular)	Stoddard solvent ^a (140 flash)	Stoddard solvent ^b	Stoddard solvent ^c	Stoddard solvent ^d
Alkanes (paraffins)	30–50 (48 average)	60.8	34.9	41.6	47.7
n-Nonane					
n-Decane					
Methylnonanes					
2,6-Dimethyloctane					
n-Undecane					
Dodecanes					
Terdecanes					
Others					
Cycloalkanes (cycloparaffins)	30–40 (38 average)	35.7		39.5	37.6
Monocycloparaffins		24.5	34.9	27.9	26
Trimethylcyclohexane					
tert-Butylcyclohexane					
n-Butylcyclopentane					
n-Butylcyclohexane					
Other Cycloparaffins					
Dicycloparaffins		11.2	5	11.6	11.6
Tricycloparaffins			0.4	0.00	
Acenaphthenes			0.4		

Table E-2.b. Possible Formulations of Stoddard Solvent (Percent) (continued)

Hydrocarbons	Stoddard solvent ^a (regular)	Stoddard solvent ^a (140 flash)	Stoddard solvent ^b	Stoddard solvent ^c	Stoddard solvent ^d
Aromatics	10–20 (14.1 average)	3.4		18.9	
Alkylbenzenes	14	3.03	22	17.6	14.1
Dimethylethylbenzenes					
n-Propylbenzene					
Ethyltoluenes					
1,2,4-Trimethylbenzene					
Other aromatics			1.1		
Other benzenes	0.1	0.07			0.1
Indans/Tetralins	<1	0.3	1.8	1.3	0.5
Indenes			0.1		
Naphthalenes			0.2		
Acenaphthalenes			0.3		
Tricyclicaromatics			0.1		

^a Adapted from Air Force (1989)

^b Adapted from American Petroleum Institute (1976)

^c Adapted from Suntech Group (1978); API 1978

^d Adapted from Carpenter et al. (1975); this paper also includes a mass spectral analysis of components by carbon number within a hydrocarbon class, e.g., C₈ alkanes

APPENDIX E

Table E-2.c. Physical and Chemical Properties of Stoddard Solvent

Property	Information	Reference
Molecular weight	144 (mean); 135–145 (range)	Air Force 1989b; Carpenter et al. 1975b
Color	Clear, colorless	Sax and Lewis 1989
Physical state	Liquid	Sax and Lewis 1989
Melting point	No data	
Boiling point	154–202 °C 160–199 °C	Air Force 1989b Coast Guard 1985
Density at 20 °C	0.78 g/mL	NIOSH 1990
Odor	Similar to kerosene	NIOSH 1990
Odor threshold	0.9 ppm (5.1 mg/m ³) 2 mg/m ³	Carpenter et al. 1975b Hastings et al. 1984
Solubility:		
Water	Insoluble	McDermott 1975
Organic solvents	Absolute alcohol, benzene, ether, chloroform, carbon tetrachloride, carbon disulfide	Sax and Lewis 1989
Partition coefficients:		Air Force 1989b
Log K _{ow}	3.16–7.06	Air Force 1989b
Log K _{oc}	2.85–6.74	
Vapor pressure at 25 °C	4–4.5 mm Hg	McDermott 1975
Henry's law constant at 20 °C	4.4x10 ⁰ atm·m ³ /mol	Air Force 1989b
Autoignition temperature	232 °C	Sax and Lewis 1989
Flashpoint	37.8–60.0 °C 38–43 °C	Air Force 1989b Sax and Lewis 1989
Flammability limits in air at 25 °C	0.9–6.0	Carpenter et al. 1975b
Conversion factors: at 25 °C and 760 mm	1 mg/L = 174.5 ppm 1 ppm = 5.73 mg/m ³	Carpenter et al. 1975b Air Force 1989b
Explosive limits		McDermott 1975
Lower limit	0.9%	
Upper limit	6%	

APPENDIX E

Table E-3a. Chemical Identity, Composition and Chemical Physical Properties of JP-4^a

Character	Information	Reference
Chemical Name	JP-4	OHM/TADS 1985
Synonym(s)	Jet Fuel-4	OHM/TADS 1985
Registered Trade Name(s)	NIL-T-5624-L-Amd. 1; wide cut; JP-4 military (gasoline type)	Air Force 1990c; Dickson and Woodard 1987; Dukek 1978; IARC 1989
Identification Numbers:		
CAS Registry	50815-00-4	OHM/TADS 1985
NIOSH RTECS	NY9340000	RTECS 1991
EPA Hazardous Waste	No data	
OHM/TADS	7217071	OHM/TADS 1985
DOT/UN/NA/IMCO shipping	1863	CHRIS 1986
HSDB	No data	
NCI	No data	

^aJP-4 is a mixture of C-4 to C-16 hydrocarbons with an approximate distribution by chemical class of 32% straight alkanes, 31% branched alkanes, 16% cycloalkanes, and 21% aromatic hydrocarbons.

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data Systems; RTECS = Registry of Toxic Effects of Chemical Substances

APPENDIX E

Table E-3.b. Typical Hydrocarbon Composition of JP-4 Jet Fuel

Compound	Weight Percent
Straight Alkanes	32
Butane	0.12
Pentane	1.06
Hexane	2.21
Heptane	3.67
Octane	3.80
Nonane	2.25
Decane	2.16
Undecane	2.32
Dodecane	2.00
Tridecane	1.52
Tetradecane	0.73
Pentadecane	—
Hexadecane	—
Heptadecane	—
Octadecane	—
Isoalkanes	31
Isobutane	0.66
2,2-Dimethylbutane	0.10
2-Methylpentane	1.28
3-Methylpentane	0.89
2,2-Dimethylpentane	0.25
2-Methylhexane	2.35
3-Methylhexane	1.97
2,2,3,3-Tetramethylbutane	0.24
2,5-Dimethylhexane	0.37
2,4-Dimethylhexane	0.58
3,3-Dimethylhexane	0.26
2,2-Dimethylhexane	0.71

APPENDIX E

Table E-3.b. Typical Hydrocarbon Composition of JP-4 Jet Fuel (continued)

Compound	Weight Percent
2-Methylheptane	2.70
4-Methylheptane	0.92
3-Methylheptane	3.04
2,5-Dimethylheptane	0.52
2,4-Dimethylheptane	0.43
4-Ethylheptane	0.18
4-Methyloctane	0.86
2-Methyloctane	0.88
3-Methyloctane	0.79
2-Methylundecane	0.64
2,6-Dimethylundecane	0.71
2,4,6-Trimethylheptane	—
4-Methyldecane	—
2-Methyldecane	—
2,6-Dimethyldecane	—
2-Methylundecane	—
2,6-Dimethylundecane	—
Cycloalkanes	16
Methylcyclopentane	1.16
Cyclohexane	1.24
trans-1,3-Dimethylcyclopentane	0.36
cis-1,3-Dimethylcyclopentane	0.34
cis-1,2-Dimethylcyclopentane	0.54
Methylcyclohexane	2.27
Ethylcyclopentane	0.26
1,2,4-Trimethylcyclopentane	0.25
1,2,3-Trimethylcyclopentane	0.25
cis-1,3-Dimethylcyclohexane	0.42

APPENDIX E

Table E-3.b. Typical Hydrocarbon Composition of JP-4 Jet Fuel (continued)

Compound	Weight Percent
1-Methyl-3-ethylcyclohexane	0.17
1-Methyl-2-ethylcyclohexane	0.39
Dimethylcyclohexane	0.43
1,3,5-Trimethylcyclohexane	0.99
1,1,3-Trimethylcyclohexane	0.48
1-Methyl-4-ethylcyclohexane	0.48
n-Butylcyclohexane	0.70
Propylcyclohexane	—
Hexylcyclohexane	—
Heptylcyclohexane	—
Aromatic Hydrocarbons	21
Benzene	0.50
Toluene	1.33
Ethylbenzene	0.37
m-Xylene	0.96
p-Xylene	0.35
o-Xylene	1.01
Isopropylbenzene	0.30
n-Propylbenzene	0.71
1-Methyl-3-ethylbenzene	0.49
1-Methyl-4-ethylbenzene	0.43
1,3,5-Trimethylbenzene	0.42
1-Methyl-2-ethylbenzene	0.23
1,2,4-Trimethylbenzene	1.01
1,3-Diethylbenzene	0.46
1,4-Diethylbenzene	—
1-Methyl-4-propylbenzene	0.40
1,3-Dimethyl-5-ethylbenzene	0.61

APPENDIX E

Table E-3.b. Typical Hydrocarbon Composition of JP-4 Jet Fuel (continued)

Compound	Weight Percent
1-Methyl-2-isopropylbenzene	0.29
1,4-Dimethyl-2-ethylbenzene	0.70
1,2-Dimethyl-4-ethylbenzene	0.77
1,2,3,4-Tetramethylbenzene	0.75
1-Ethylpropylbenzene	—
1,2,4-Triethylbenzene	—
1,3,5-Triethylbenzene	—
Phenylcyclohexane	—
1-tert-Butyl-3,4,5-trimethylbenzene	—
n-Heptylbenzene	—
Naphthalene	0.50
2-Methylnaphthalene	0.56
1-Methylnaphthalene	0.78
2,6-Dimethylnaphthalene	0.25
Biphenyl	—
1-Ethylnaphthalene	—
2,3-Dimethylnaphthalene	—
n-Octylbenzene	—

APPENDIX E

Table E-3.c. Physical and Chemical Properties of JP-4^a

Property	Information	Reference
Molecular weight	Not applicable ^b	
Color	Colorless to straw colored	CHRIS 1986; Martel 1992
Physical state	Liquid	CHRIS 1986
Melting point	-46 °C -40–72 °C	OHMTADS 1985 ITC 1985
Boiling point (1 atm)	50–270 °C 90–300 °C 45–280 °C	Air Force 1989b ITC 1985 Dickson and Woodward 1987
Density at 15 °C	751–802 kg/m ³ (specification)	
Odor	Like gasoline and/or kerosene	
Odor threshold:		
Water	No data	
Air	1 ppm	CHRIS 1986
Solubility:		
Water at 20 °C	57 mg/L	CRC 1984
Organic solvents	Since many of the components are organic solvents, the fuel is generally miscible with organic solvents	ITC 1985
Partition coefficients:		
Log K _{ow}	Major components range from 3 to 4.5	ITC 1985
Log K _{oc}	No data	
Vapor pressure at 20 °C	91 mm Hg	Air Force 1989b
Henry's law constant	1.00x10 ⁻⁴ –1.00x10 ¹ atm·m ³ /mol	Air Force 1989b
Autoignition temperature	246 °Cd	CRC 1984
Flashpoint	-23–1 °C	NFPA 1986
Flammability limits	1.3% lower; 8.0 upper	NFPA 1986
Explosive limits	No data	

^a JP4, or jet propellant-4, is a mixed compound composed primarily of hydrocarbons (i.e., alkanes, cycloalkanes, alky-benzenes, indan/tetralins, and Naphthalenes).

^b Jet fuels are blends prepared to meet certain gross property specifications. Most characteristic data only reflect gross properties covered in the specifications. Proportions and values vary with the type of crude oil from which the final fuel is derived and the refining process used.

APPENDIX E

Table E-4.a. Chemical Identity of Fuel Oils

Character	Information		
Chemical Name	Fuel oil No. 1 ^a	Fuel Oil No. 2 ^b	Fuel oil No. 6 ^c
Synonym(s)	Kerosene, coal oil kerosine, range oil, straight run kerosene, distillate fuel oils light, furnace oil no. 1, Deobase [®] , JP-5, JP-1, range oil	API no. 2 fuel oil, gas oil, home heating oil no. 2, number 2 burner oil, diesel fuel, furnace oil no. 2	No. 6 fuel oil, Bunker C
Registered Trade Name(s)	Deobase [®]		
Identification Numbers:			
CAS Registry	8008-20-6	68476-30-2	68553-00-4
NIOSH RTECS	OA5500000	HZ1800000	LS8940000
EPA Hazardous Waste	No data	No data	No data
OHM/TADS	7217063	No data	No data
DOT/UN/NA/IMCO	UN 1223, IMO 3.3	No data	No data
shipping	632	No data	No data
HSDB	No data	C54795	No data
NCI			

^a Fuel oil #1 is a mixture of C-9 through C-16 hydrocarbons primarily containing approximately 64% aliphatic hydrocarbons, 1–2% olefinic hydrocarbons, and 35% aromatic hydrocarbons.

^b Fuel oil #2 is a mixture of C-11 to C-20 hydrocarbons.

^c Fuel oil #6 is 25% aromatics, 15% paraffins, 45% naphthenes, and 15% non-hydrocarbon compounds

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute
NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data Systems; RTECS = Registry of Toxic Effects of Chemical Substances

Source: ATSDR Toxicological Profile for Fuel Oils, 1995.

APPENDIX E

Table E-4b. Analysis of Fuel Oils^a

Hydrocarbon type	Volume %		
	Fuel oil no. 1	Fuel oil no. 2	Fuel Oil no. 6
Paraffins (<i>n</i> - and iso-)	52.4	41.3	5.9
Monocycloparaffins	21.3	22.1	3.9
Bicycloparaffins	5.1	9.6	3.4
Tricycloparaffins	0.8	2.3	2.9
Other cycloparaffins	-	-	5.0
Total saturated hydrocarbons	79.7	75.3	21.1
Olefins	No data	No data	No data
Alkylbenzenes	13.5	5.9	1.9
Indans/tetralins	3.3	4.1	2.1
Dinaphthenobenzenes/indenes	0.9	1.8	2.6
Naphthalenes	2.8	8.2	2.6
Biphenyls/acenaphthenes	0.4	2.6	3.1
Fluorenes/acenaphthylenes	No data	1.4	7.0
Phenanthrenes	No data	0.7	11.6
Other aromatic hydrocarbons	No data	No data	57.8
Total aromatic hydrocarbons	23.6	24.7	78.9

^a Derived from IARC 1989; provided by the American Petroleum Institute

APPENDIX E

Table E-4c. Physical and Chemical Properties of Fuel Oils

Property	Fuel oil no. 1	Fuel oil no. 2	Fuel oil no. 6
Molecular weight	No data	No data	No data
Color	Pale Yellow ^b ; Colorless to brown ^{c,d}	Colorless to brown ^c	Colorless to brown
Physical state	Liquid ^c	Liquid ^c	Liquid
Melting point	-45.6 °C	-29 °C	No data
Boiling point	175–325 °C ^b ; 200–260 °C ^d	160–360 °C ^f ; 282–338 °C ^d	151–588 °C
Density at 15 °C at 20 °C	0.810–0.9360 g/mL ^c 0.80 g/mL ^{e,f}	No data 0.8700–0.9500 °C	No data No data
Odor	Kerosene-like ^c	Kerosene-like ^c	Kerosene-like
Odor threshold (ppm)	0.082 ^f ; 1 ^d	No data	No data
Solubility: Water at 20 °C Organic solvents	≈5 mg/L ^c Miscible with other petroleum solvents ^b	≈5 mg/L ^c No data	≈5 mg/L No data
Partition coefficients: Log K _{ow} Log K _{oc}	3.3–7.06 ^c 3.0–6.7 ^c	3.3–7.06 ^c 3.0–6.7 ^c	3.3–7.06 3.0–6.7
Vapor pressure at 21 °C	2.12–26.4 mm Hg ^c	2.12–26.4 mm Hg ^c	No data
Henry's law constant at 20 °C - atm·m ³ /mol	5.9x10 ⁻⁵ –7.4 ^c	5.9x10 ⁻⁵ –7.4 ^c	No data
Autoignition temperature	229 °C ^d	257 °C ^d	No data
Flashpoint (close cup)	38 °C ^{c,d}	58 °C ^d	No data
Flammability limits (% volume in air)	0.7–5% ^d	0.6–7.5% ^d	No data
Conversion factors	No data	No data	No data
Explosive limits	0.7–5% ^b	No data	No data

^aValues listed are specifications required or general characteristics of each class of fuel oils

^bHSDB 1991

^cAir Force 1989

^dCoast Guard 1985

^eIARC 1989

Source: ATSDR toxicological profile for Fuel Oils

APPENDIX E

Table E-5.a. Chemical Identity of Mineral-Based Crankcase Oil

Character	Information	Reference
Chemical Name	Mineral-based crankcase oil	ATSDR 1997c
Synonym(s)	API 79-7; API service classification SAE 30 automotive motor oil; monograde automotive engine oil; multigrade automotive engine oil; marine engine oil; base engine oil; monograde diesel oil; railway diesel oil; marine diesel oil	ATSDR 1997c
Registered Trade Name(s)	Not applicable	
Chemical Formula	Not applicable	
Chemical Structure	Not applicable	
Identification Numbers:		
CAS Registry	8002-05-9	IARC 1984
NIOSH RTECS	No data	
EPA Hazardous Waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	No data	
HSDB	No data	
NCI	No data	

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute
 NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data Systems; RTECS = Registry of Toxic Effects of Chemical Substances

APPENDIX E

Table E-5.b. Concentration of Components in Used Mineral-Based Crankcase Oil^a

Component	Median concentration (ppm)
Arsenic	5
Barium	48
Cadmium	3
Chromium	6.5
Lead	240
Zinc	480
Dichlorodifluoromethane	20
Trichlorotrifluoroethane	160
1,1,1-Trichloroethane	200
Trichloroethylene	100
Tetrachloroethylene	106
Benzene	20
Toluene	380
Xylene	550
Benz(a)anthracene	12
Benzo(a)pyrene	10
Naphthalene	330
PCBs	5

^a Environmental contamination from mineral-based crankcase oil is more likely to be from used crankcase oil than for the fresh products. Used oil is significantly contaminated with heavy metals and polycyclic aromatic hydrocarbons that are insignificant in the unused products. TPH results do not yield values for these contaminants, but the table is provided for informational purposes.

Source: ABB-Environmental Service, Inc. 1990

APPENDIX E

Table E-5.c. Physical and Chemical Properties of Mineral-Based Crankcase Oils

Property	Information	References
Molecular weight	No data	
Color	Yellow brown	DOE 1989
Physical state	Liquid, oily	DOE 1989
Melting point	-34.4 °C	DOE 1989
Boiling point	360 °C	DOE 1989
Density at 20 °C	Not applicable	
Odor	Lube oil odor	DOE 1989
Odor threshold (ppm)	No data	
Solubility		
Water at 20 °C	Insoluble	DOE 1989
Organic solvents	No data	
Partition coefficients:		
Log K_{ow}	No data	
Log K_{oc}	No data	
Vapor pressure at 21 °C	No data	
Henry's law constant at 20 °C - atm-m ³ /mol	No data	
Autoignition temperature	≥ 135 °C	DOE 1989
Flashpoint (close cup)	≥ 163 °C	DOE 1989
Flammability limits (% volume in air)	No data	
Conversion factors	No data	
Explosive limits	No data	

Source: ATSDR. 1997. Toxicological profile for mineral-based crankcase oil. Agency for Toxic Substances and Disease Registry. Atlanta, GA.

APPENDIX E

Table E-6a. Chemical Identity of Mineral Oil^a

Character	Information	Reference
Chemical Name	Mineral Oil	RTECS 1995
Synonym(s)	Paraffin oils, Heavy mineral oil, Light mineral oil, Liquid paraffin, Aliphatic petroleum hydrocarbons, Liquid Vaseline, Paraffins, Paroleine, Liquid Petrolatum, White Mineral Oil, White Oils	RTECS 1995; ATSDR 1997b
Registered Trade Name(s)	Nujol, Thermia C, ADEPSINE OIL, ALBOLINE, Balneol, BAYOL F, Bayol 55, Blandlube, Crystosol, Drakeol, FLEXON 845, Fonoline, GLYMOL, Crystosol, IRGAWAX 361, KAYDOL, Kondremul, MagieSol 44, Molol, Neo-Cultol, Parol, Peneteck, Penreco, Perfecta, Petrogalar, PRIMOL D, Primol 355, Protopet, SAXOL, SHELLFLEX 371N, SUNPAR 150, Tech Pet F, ULTROL 7, UVASOL	
Identification Numbers:		
CAS Registry	8020-83-5; 8012-95-1	RTECS 1995
NIOSH RTECS	LX3300000	RTECS 1995
EPA Hazardous Waste	No data	
OHM/TADS	7217073	OHM/TADS 1991
DOT/UN/NA/IMCO shipping	UN1203, UN1257	RTECS 1995
HSDB	No data	
NCI	No data	

^a Mineral oil refers to classes of petroleum hydrocarbons whose origin is petroleum distillation streams. Light paraffinic (naphthenic) distillate contains C₁₅-C₃₀ hydrocarbons; heavy paraffinic (naphthenic) distillate contains C₂₀-C₅₀ hydrocarbons; white mineral oil contains C₁₅-C₅₀ hydrocarbons, and petrolatum and most residual oils contains >C₂₅ hydrocarbons. Source: IARC 1984.

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data Systems; RTECS = Registry of Toxic Effects of Chemical Substances

APPENDIX E

Table E-6.b. Physical and Chemical Properties of Mineral Oil^a

Property	Information	Reference
Molecular weight	No data	
Color	Clear	HSDB 1998
Physical state	Liquid	HSDB 1998
Melting point	No data	
Boiling point	360°C	HSDB 1998
Density at 20/4 °C	0.875–0.905	HSDB 1998
Odor	Like burned lubricating oil	HSDB 1998
Odor threshold: Water Air	No data	
Solubility: Water at 25 °C Organic solvents	Insoluble Soluble	HSDB 1998 HSDB 1998
Partition coefficients: Log K _{ow} Log K _{oc}	No data No data	
Vapor pressure at 20/30 °C	No data	
Henry's law constant at 24.8 °C	No data	
Autoignition temperature	500–700°F	HSDB 1998
Flashpoint	135°C (closed cup) 193°C (open cup)	HSDB 1998 HSDB 1998
Flammability limits in air	No data	
Conversion factors: ppm (v/v) to mg/m ³ in air at 25 °C	1 ppm (v/v) = 3.96 mg/m ³	
mg/m ³ to ppm (v/v) in air at 25 °C	1 mg/m ³ = 0.25 ppm (v/v)	
Explosive limits	No data	

^a Mineral oil refers to classes of petroleum hydrocarbons whose origin is petroleum distillation streams. Light paraffinic (naphthenic) distillate contains C₁₅–C₃₀ hydrocarbons; heavy paraffinic (naphthenic) distillate contains C₂₀–C₅₀ hydrocarbons; white mineral oil contains C₅₀ hydrocarbons, and; petrolatum and most residual oils contains >C₂₅ hydrocarbons. Source: IARC 1984.
Source: HSDB. 1998. Hazardous Substances Database. Environmental Protection Agency, available through National Library of Medicine, MEDLARS, Washington, DC.

INDEX

Acenaphthene	114, 117, 119
Acenaphthylene	114, 117, 119
Alcohols	21
Aliphatic fractions	32, D-1
Aliphatic hydrocarbons	22, 41
Alkanes	21, 23, 32, 37, 156, 173, 175, B-1
alkanes, n-	13, 34, 71, 73, 79, 98
Alkenes	20, 21, 122, 124, 173
Alkyl PAHs	23
Alkyl aromatics, n-	73
Alkyl benzenes	114
Alkyl tertiary butyl ethers	20
Alkylbenzenes	22, 114
Anthracene(s)	119, 120, 122
Aromatic fractions/hydrocarbons	21-23, 32, 156, D-1
Aromatics	23, 155, D-1
Asphalt	24
ASTM	96
Automotive gasoline (see gasoline)	
Aviation fuels (see Jet Fuels)	21, 40
Barium	52
Barrel of crude	42, 45
Benzene	4, 5, 7, 11, 16, 17, 37, 40, 41, 52, 54, 65, 71-73, 76, 80, 84, 85, 94, 97, 98, 100, 101, 104, 105, 110, 137, 141, 142, 145-147, 152, 153, 155, 160, 165, 171, 181, 183-186, 189
Benzene rings	13
Benzo(a)anthracene	97, 100, 119, 122
Benzo(a)pyrene	5, 37, 97, 98, 100, 119, 122, 149
Benzo(b)fluoranthene	97, 100, 119
Benzo(k)fluoranthene	97, 100
Benzo(e)pyrene	119
Benzo(g,h,i)perylene	119
Benzo(j)fluoranthene	119
Benzo(k)fluoranthene	119
Biphenyls	114, 117, 168
Branched alkanes	173, 175
BTEX	16, 37, 84, 85, 97, 100, 104, 105, 110, 147, 149, 151, 152, 154-156, 162, 165, 180, 181, 185, 186, 188, 190
Butadiene	40
Butane	40, 71
Butylbenzene, n-	114
Butylbenzenes	110, 153
Butylcyclohexane, t-	150, 152, 153
Butylenes	40
Chromatography (see GC)	11
Chrysene	97, 100, 119
Crankcase oils/motor oils (see Mineral spirits and Oils)	3, 23, E-1
Crude oil	1, 9, 10, 18, 20, 40-42, 47, 53

INDEX

Crude oil production	17, 42, 47
Cumene (isopropylbenzene)	99, 110, 153
Cyclic alkanes	173, 175
Cycloalkanes	20-23, 148, 156, 173
Cyclohexane	41, 124, 125, 127, 150, 152, 153, 173
Cyclopentane	41, 122, 127, 173
Decane, n-	129, 150, 152, 153, 173
Dibenzo(a,h)anthracene	97, 100, 119, 122
Diesel fuels	7, 11, 22, 60, 67, 84, 97, 139
Diesel fuel oil #1	22
Diesel fuel #2	22, 139
Diesel fuels, marine	139
Diesel range organics (DRO)	30
Dimethylbutanes	122, 127, 173
2,3-dimethylbutane	124
Dimethylcyclohexane	150, 152, 153
Dimethylnaphthalenes	114
Distillate fuels	139
DNAPLs (denser non-aqueous phase liquids)	67, 70
Dodecane, n-	129
Eicosdecane, n-	175
EPA Method 1664	25
EPA Method 3611	32
EPA Method 3630	32
EPA Method 413.1	24
EPA Method 413.2	24
EPA Method 418.1	11, 24, 25, 30, 33
EPA Method 8015 (modified)	11, 12, 33
EPA Methods 8020/8015, modified	32
Equivalent carbon number index (EC)	80, 98
Ethane	40
Ethanol (ethyl alcohol)	20
Ethyl alcohol	20
Ethylbenzene	5, 16, 17, 71-73, 85, 97, 101, 104, 105, 110, 114, 160, 165, 183, 186
Ethylene	40, 41
Ethylene dichloride	20
Ethylene dibromide	20
Flame ionization detection (FID)	11, 32, 35
Fluoranthene	101, 119, 122
Fluorene(s)	119, 120, 122
Fraction approach, ATSDR	15, 99
Fuel oils	17, 20, 40-42, 59, 60, 67, 73, 84, 139, 140, 183, 188, E-1
Fuel oil #1	22, 129, 139, 140
Fuel oil #2	22, 72, 139, 140
Fuel oil #4	139
Fuel oil #6	22, 23
Fuel oils, heavy	97, 140
Fuel oils, light	25, 97
Fuel oils, residual	23

INDEX

Fuels	42, 84
Gas chromatography (GC)	11, 25, 30, 33, 34, 37, 98
GC/FID	30, 32, 34, 35
GC/MS	34, 35
Gasolines	3, 5, 7, 11, 20, 22, 25, 30, 34, 37, 38, 40, 41, 54, 59, 60, 65, 69, 71-73, 79, 84, 85, 95, 97, 141, 142, 160, 178, 183, 188, 193
Gasoline fumes	57
Gasoline, automotive	10, 20, E-1
Gasoline, mixtures	85
Gasoline, tanks	65
Gasoline, unleaded	142
Glycols	21
GRO (gasoline range organics)	30
Heating oil	41, 56
Henry's law constant	71, 78, 79, 99
Heptadecane, n-	175
Heptane, n-	124, 125, 173
Hexadecane	129
Hexanedecane, n-	156
Hexane (see n-hexane)	32, 33, 76, 99, 122, 124, 125, 127, 173
2,5-Hexanedione	155
Hexanoic acid	155
Hexanols	
1-Hexanol	155
2-Hexanol	155
3-Hexanol	155
Hexanone	
2-Hexanone	155
5-Hydroxy-2-hexanone	155
HMT (hazardous material transport)	54
HSSM	76
Hydraulic fluids (mineral based)	32, 134, 183, 188
Hydrocarbon fractions	32
Hydrocarbon Spill Screening Model (HSSM)	76
Indan	114
Indeno(1,2,3-cd)pyrene	97, 100, 119
Index of concern	181, 227
Infrared (IR) spectrometry	25
Isoalkanes	20
Isopropylbenzene (cumene)	114, 115, 153
Jet fuels	10, 17, 20, 21, 84, 97, 135, 137-139, 175, 183, 188, 191, E-1
Jet A	21, 138
JP-4	21, 22, 85, 95, 137, 138, E-1
JP-5	21, 129, 130, 132, 137-140, 158, 161, 175, 191
JP-7	21, 101, 129, 130, 132, 137, 138, 161, 175, 191
JP-8	21, 129, 130, 132, 137, 175, 191
Kerosenes	5, 21, 22, 42, 72, 97, 129, 130, 132, 137-140, 160, 175
Kerosene, straight run	139
Kerosenes, jet fuel	42, 137

INDEX

Ketones	21
Lead	21, 52
Leaking underground storage tanks (LUST)	17
Linear alkanes	21
Liquified petroleum gas (LPG)	40, 42
LNAPLs (lighter non-aqueous phase liquids)	67, 70
LOAELs	102, 103, 105, 110, 227, 231, B-1, B-2
Lubricants	42, 59
LUST (see leaking underground storage tank systems, see also UST)	
MADEP	12, 32, 97-100
Mass spectrometry (MS)	35
Methanol (methyl alcohol)	20
Methyl-tert-butyl ether (MTBE)	95
Methylcyclohexane	124, 125, 150, 152, 153, 173
Methylcyclopentane	124, 127
Methylene chloride	33
Methylethylbenzene	110, 114
Methylindans	114
Methylnaphthalenes	168
1-Methylnaphthalene	114, 117, 168
2-Methylnaphthalene	114, 151, 153, 155
Methylpentanes	122, 173
2-Methylpentane	124, 127
3-Methylpentane	124, 127
Microwave extraction	33
Mineral oil	101, E-1
Mineral spirits	21
Mineral-based crankcase oils	23, 183, 188
Mineral-based hydraulic fluid	132
Mineral-based oils	23
Minimal Risk Levels (MRLs)	13, 93, 94, 96, 100, 103, 105, 110, 180, A-1
Mixtures	96
Monomethylnaphthalenes	114, 147, 151
Motor oil	23, 69
Motor oil, synthetic	23
Motor oils, used	23
MRLs (see minimal risk levels)	
MTBE (see methyl-tert-butyl ether)	
n-Alkane (see alkanes)	
n-Hexane	4, 5, 17, 25, 37, 98, 99, 101, 122, 124, 125, 127, 148, 150, 152, 153, 155, 157, 160, 173, 184
Naphtha	20-22, 34
Naphthalene	94, 99, 101, 114, 115, 119, 151, 156
Naphthenes	4, 23, 152
Naphthenes, C6-C10	150, 153
Naphthenes, fuel oil #6	23
NAPLs (non-aqueous phase liquids)	84
Nonadecane, n-	175
Nonane, n-	98, 129, 173
Non-hydrocarbon compounds	23

INDEX

Octadecane, n-	175
Octane, n-	32, 34, 124, 173
Oil production wastes	54
Oils	
Oil, bulk	69
Oil, crude	78
Oil, mineral-based crankcase	17, 23, 24, 132
Oil, used	53-55
Oil, used motor/automotive	23, 47, 65
Oil, used, as waste	53
Oil, used, mineral-based	134
Oil, used, motor/crankcase	59, 75, 134, 144
Oil, used, recycled	53
Oils, synthetic	23
Olefinic hydrocarbons	22
Olefins	41
PAHs	22, 23, 59, 67, 73, 74, 94, 97, 114, 119, 120, 122
PAHs, carcinogenic	37
PAHs, noncarcinogenic	37
Paraffins	23
PCBs	56
Pentadecane	129
Pentane, n-	34, 122, 173
Pentylbenzene, n-	114
Pentylcyclopentane	129
Pesticides	3
Petroleum	59
Petroleum hydrocarbons ..	2, 9, 10, 16-18, 25, 32, 37, 47, 57, 69, 74, 75, 80, 95, 99, 102, 114, 129, 134, 147, 159-161, 178, 183-185, 187-189
Petroleum products	39, E-1
Petroleum wastes	38, 52, 54
Petroleum, crude	139
Phenanthrenes	52, 119
Phenol	75
Photo ionization detector (PID)	32
Polycyclic aromatic hydrocarbons (see PAHs)	
Propane	71
Propylbenzene, n-	110
Propylene	40, 41
Public health statement	1
Purge-and-trap gas chromatography (GC)	11, 30, 32, 33
Pyrenes	37, 119
Recovered oil	53
Residual fuels	139
RfC (reference concentration)	94, 97, 229, 231
RfD (reference dose)	94, 97, 230, 231, B-2
Risk-Based Corrective Action (RBCA)	10, 12, 13, 78, 81, 85, 96, 194
Risk-Based Screening Level (RBSL)	81
RQ (reportable quantity)	53

INDEX

Solid phase extraction (SPE)	33
Solvent extraction	33
Sonication extraction	33
Soxhlet extraction	33
SSTL (site-specific target level)	81
Stoddard solvent	21, 34, 129, 143, 183, 188, E-1
Straight-chain pentane	41
Substituted cycloalkanes	173
Sulfur	21
Supercritical fluid extraction (SFE)	33
Tetradecane	129
Tetraethyl-lead	20
TOG (total oil and grease)	24
Toluene	4, 16, 17, 37, 40, 54, 67, 71-73, 75, 80, 84, 85, 97, 99, 101, 104, 105, 110, 145, 147, 152, 153, 155, 160, 165, 181-183, 186
Total Petroleum Hydrocarbons, defined	1, 9
Total Petroleum Hydrocarbons Criteria Working Group (TPHCWG)	10-13, 18, 24, 30, 57, 79, 98-100, 102, 134, 178
Total recoverable oil and grease (TOG, TROG)	24
Total recoverable petroleum hydrocarbons (TPH, TRPH, or TPH-IR)	25
TPH, defined	1, 9
Transport models	80
Tridecane, n-	129
Trimethylbenzene	110, 114, 152, 153
1,3,5-trimethylbenzene	115
Trimethylcyclohexane	150, 152, 153
Trimethylpentanes	124, 173
TROG (total recoverable oil and grease)	24
Undecane, n-	129
Underground storage tank systems (UST)	10, 30, 33, 54-56, 60, 65, 194
UST (underground storage tank systems)	
Waste oil	7
Weight of evidence (WOE)	110
White spirits	21, 99
Xylene	4, 16, 40, 54, 71-73, 85, 97, 101, 104, 105, 110, 152, 153, 160, 165, 183, 186
Mixed xylenes	105, 186
m-Xylene	105
p-Xylene	105, 181

