

### 3. CHEMICAL AND PHYSICAL INFORMATION

#### 3.1 CHEMICAL IDENTITY

Gasoline is a refined product of petroleum consisting of a mixture of hydrocarbons, additives, and blending agents. The composition of gasolines varies widely, depending on the crude oils used, the refinery processes available, the overall balance of product demand, and the product specifications. The typical composition of gasoline hydrocarbons (% volume) is as follows: 4-8% alkanes; 2-5% alkenes; 25-40% isoalkanes; 3-7% cycloalkanes; 1-4% cycloalkenes; and 20-50% total aromatics (0.5-2.5% benzene) (IARC 1989). Additives and blending agents are added to the hydrocarbon mixture to improve the performance and stability of gasoline (IARC 1989; Lane 1980). These compounds include anti-knock agents, anti-oxidants, metal deactivators, lead scavengers, anti-rust agents, anti-icing agents, upper-cylinder lubricants, detergents, and dyes (IARC 1989; Lane 1980). At the end of the production process, finished gasoline typically contains more than 150 separate compounds although as many as 1,000 compounds have been identified in some blends (Domask 1984; Mehlman 1990). Information regarding the chemical identity of gasoline is located in Table 3-1.

#### 3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties for the gasoline mixture is located in Table 3-2. In cases where data are not available for gasoline, ranges are given to indicate the different values for the individual components.

## CHEMICAL AND PHYSICAL INFORMATION

**TABLE 3-1. Chemical Identity of Gasoline**

Characteristic	Information	Reference
Chemical name	Gasoline	RTECS 1990
Synonyms	Casing head gasoline; motor fuel; motor spirit; natural gasoline; petrol	HSDB 1993
Registered trade name(s)	No data <sup>a</sup>	
Chemical formula	No data <sup>a</sup>	
Chemical structure	No data <sup>a</sup>	
Identification numbers:		
CAS registry	8006-61-9	RTECS 1990; Sax and Lewis 1989
NIOSH RTECS	LX3300000	RTECS 1990; SANSS 1986; Sax and Lewis 1989
EPA hazardous waste OHM/TADS	No data 7217073	OHM/TADS 1991; SANSS 1986
DOT/UN/NA/IMCO shipping	UN1203, UN1257	RTECS 1990
HSDB	No data	
NCI	No data	

<sup>a</sup>Gasoline is a mixed compound consisting of hydrocarbons, blending agents, and additives.

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 System; RTECS = Registry of Toxic Effects of Chemicals Substances; SANSS = Structure and Nomenclature Search System

## CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2. Physical and Chemical Properties of Gasoline

Property	Information	Reference
Molecular weight	108 <sup>a</sup>	Anonymous 1989
Color	Colorless to pale brown or pink	Sax and Lewis 1989; Weiss 1986
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	Budavari et al. 1989; OHM/TADS 1991; Sax and Lewis 1989
Density	0.7-0.8 g/cm <sup>3b</sup>	IARC 1989
Odor	Gasoline odor	Weiss 1986
Odor threshold	0.025 ppm <sup>c</sup>	Weiss 1986
Solubility: Water at 20°C	Insoluble	OHM/TADS 1991; Sax and Lewis 1989
Organic solvent(s)	Absolute alcohol, ether, chloroform, benzene	Budavari et al. 1989; Sax and Lewis 1989
Partition coefficients: Log K <sub>ow</sub>	2.13-4.87 <sup>d</sup>	Air Force 1989
Log K <sub>oc</sub>	1.81-4.56 <sup>d</sup>	Air Force 1989
Vapor pressure <sup>e</sup> at 60°C	465 mmHg	ASTM 1989
at 56°C	518 mmHg	
at 51°C	593 mmHg	
at 47°C	698 mmHg	
at 41°C	773 mmHg	
Henry's law constant: at 20°C	4.8x10 <sup>-4</sup> -3.3 m <sup>3</sup> /mol <sup>d</sup>	Air Force 1989
Autoignition temperature	280-486°C	NEPA 1986; Sax and Lewis 1989; Weiss 1986
Flashpoint	-46°C	Sax and Lewis 1989
Flammability limits	1.4-7.4%	Weiss 1986

**TABLE 3-2. Physical and Chemical Properties of Gasoline (*continued*)**

Property	Information	Reference
Conversion factors	No data	
Explosive limits	1.3-6.0%	Budavari et al. 1989; Sax and Lewis 1989

<sup>a</sup>Average molecular weight

<sup>b</sup>Temperature not specified

<sup>c</sup>Not specified whether data for air or water

<sup>d</sup>Since data are not available for gasoline, ranges are given indicating different values for the individual components.

<sup>e</sup>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 five volatility classes that vary by seasonal climatic changes. The values given for vapor pressure at the given temperatures are based on these volatility classes.

## CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-3. Major Components of Gasoline<sup>a</sup>

Component	Percentage Composition <sup>b</sup>	Component
<i>n</i> -alkanes		<u>Other possible components</u>
C <sub>5</sub>	3.0	octane enhancers
C <sub>6</sub>	11.6	methyl t-butyl ether (MTBE)
C <sub>7</sub>	1.2	t-butyl alcohol (TBA)
C <sub>9</sub>	0.7	ethanol
C <sub>10</sub> -C <sub>13</sub>	0.8	methanol
total of <i>n</i> -alkanes	17.3	antioxidants
branched alkanes		<i>N,N'</i> -dialkylphenylenediamines
C <sub>4</sub>	2.2	2,6-dialkyl and 2,4,6-trialkylphenols
C <sub>5</sub>	15.1	butylated methyl, ethyl and dimethyl phenols
C <sub>6</sub>	8.0	triethylene tetramine di(monononylphenolate)
C <sub>7</sub>	1.9	metal deactivators
C <sub>8</sub>	1.8	<i>N,N'</i> -disalicylidene-1,2-ethanediamine
C <sub>9</sub>	2.1	<i>N,N'</i> -disalicylidene-propanediamine
C <sub>10</sub> -C <sub>13</sub>	1.0	<i>N,N'</i> -disalicylidene-cyclohexanediamine
total of branched	32.0	disalicylidene- <i>N</i> -methyl-dipropylene-triamine
cycloalkanes		ignition controllers
C <sub>6</sub>	3.0	tri- <i>o</i> -cresylphosphate (TOCP)
C <sub>7</sub>	1.4	icing inhibitors
C <sub>8</sub>	0.6	isopropyl alcohol
total of cycloalkanes	5.0	detergents/dispersants
olefins		alkylamine phosphates
C <sub>6</sub>	1.8	poly-isobutene amines
total of olefins	1.8	long chain alkyl phenols
aromatics		long chain alcohols
benzene	3.2	long chain carboxylic acids
toluene	4.8	long chain amines
xylenes	6.6	corrosion inhibitors
ethylbenzene	1.4	carboxylic acids
C <sub>3</sub> -benzenes	4.2	phosphoric acids
C <sub>4</sub> -benzenes	7.6	sulfonic acids
others	2.7	
total aromatics	30.5	

<sup>a</sup>Adapted from Air Force 1989<sup>b</sup>Percent by weight

