

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of arsenic and some common inorganic and organic arsenic compounds are located in Tables 4-1 and 4-2, respectively.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of arsenic and some common inorganic and organic arsenic compounds is located in Tables 4-3 and 4-4, respectively.

Arsenic appears in Group 15 (V) of the periodic table, below nitrogen and phosphorus. Arsenic is classified chemically as a metalloid, having both properties of a metal and a nonmetal; however, it is frequently referred to as a metal. Elemental arsenic, which is also referred to as metallic arsenic, (As(0)) normally occurs as the α -crystalline metallic form, which is a steel gray and brittle solid. The β -form is a dark gray amorphous solid. Other allotropic forms of arsenic may also exist. In compounds, arsenic typically exists in one of three oxidation states, -3, +3, and +5 (Carapella 1992). Arsenic compounds can be categorized as inorganic, compounds without an arsenic-carbon bond, and organic, compounds with an arsenic-carbon bond.

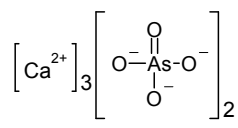
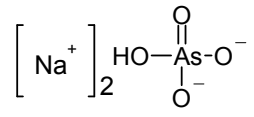
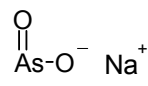
4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Arsenic and Selected Inorganic Arsenic Compounds^a

Characteristic	Arsenic	Arsenic acid	Arsenic pentoxide	Arsenic trioxide
Synonym(s)	Arsenic black; colloidal arsenic; gray arsenic, metallic arsenic	Orthoarsenic acid	Arsenic(V) oxide; arsenic acid anhydride; diarsenic pentoxide	Arsenic(III) oxide; arsenious acid; arsenious oxide; white arsenic
Registered trade name(s)	No data	Zotox; Hi-Yield Desiccant H-10; Desiccant L-10; Crab Grass Killer	No data	White Arsenic; Arsenicum Album
Chemical formula	As	H ₃ AsO ₄	As ₂ O ₅	As ₂ O ₃
Chemical structure	As	$\begin{array}{c} \text{O} \\ \parallel \\ \text{HO}-\text{As}-\text{OH} \\ \\ \text{OH} \end{array}$	[As ⁵⁺] ₂ [O ²⁻] ₅	[As ³⁺] ₂ [O ²⁻] ₃
Identification numbers:				
CAS registry	7440-38-2	7778-39-4	1303-28-2	1327-53-3
NIOSH RTECS ^b	CG0525000	CG0700000	CG2275000	CG3325000
EPA hazardous waste	D004	D004, P010	D004, P011	D004, P012
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMDG shipping	UN1558/IMDG 6.1	UN1553 (liquid)/ UN1554 (solid)/ IMDG 6.1 (liquid and solid)	UN1559/IMDG 6.1	UN1561/ IMDG 6.1
HSDB	509	431	429	419
EINECS	231-148-6	231-901-9	215-116-9	215-481-4
NCI	No data	No data	No data	No data

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-1. Chemical Identity of Arsenic and Selected Inorganic Arsenic Compounds^a

Characteristic	Calcium arsenate	Gallium arsenide	Sodium arsenate	Sodium arsenite
Synonym(s)	Calcium ortho-arsenate; arsenic acid, calcium salt	Gallium mono-arsenide	Disodium arsenate, dibasic; disodium hydrogen arsenate; arsenic acid, disodium salt	Arsenous acid, sodium salt; sodium meta-arsenite
Registered trade name(s)	Pencal; Security; Turf-Cal; Chip-Cal; SPRA-Cal	No data	No data	Atlas "A"; Penite; Kill-All; Chem-Sen 56; Chem Pels C; Progalumol Double
Chemical formula	Ca ₃ (AsO ₄) ₂	GaAs	Na ₂ HAsO ₄	NaAsO ₂
Chemical structure		Ga:As		
Identification numbers:				
CAS registry	7778-44-1	1303-00-0	7778-43-0	7784-46-5
NIOSH RTECS ^b	CG0830000	LW8800000	CG0875000	CG3675000
EPA hazardous waste	D004	D004	D004	D004
OHM/TADS	No data	No data	No data	7800057
DOT/UN/NA/IMDG shipping	UN1573/IMDG 6.1	UN 2803; Gallium/IMDG 8.0; Gallium	UN 1685/IMDG 6.1	UN1686 (aqueous solution)/UN2027 (solid)/IMDG 6.1
HSDB	1433	4376	1675	693
EINECS	233-287-8	215-114-8	231-902-4	232-070-5
NCI	No data	No data	No data	No data

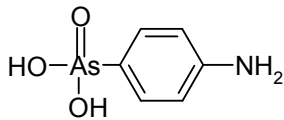
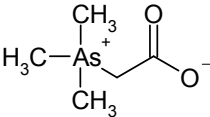
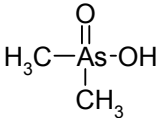
^aAll information obtained from HSDB 2007 and CHEMIDplus 2007, except where noted.

^bRTECS 2007

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/Intergovernmental Maritime Dangerous Goods Code; EINECS = European Inventory of Existing Chemical Substances; 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 Chemical Substances

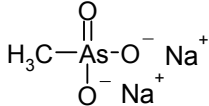
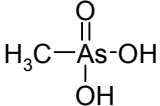
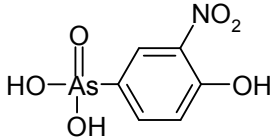
4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Chemical Identity of Selected Organic Arsenic Compounds^a

Characteristic	Arsanilic acid	Arsenobetaine	Dimethylarsinic acid
Synonym(s)	(4-Aminophenyl)arsonic acid; antoxylic acid; atoxylic acid, Pro-Gen	Arsonium, (carboxymethyl)-trimethyl-, hydroxide, inner salt	Cacodylic acid; hydroxydimethyl-arsine oxide; DMA; DMAA
Registered trade name(s)	No data	No data	510; Arsan; Phytar 560; Rad-E-Cate 35
Chemical formula	C ₆ H ₈ AsNO ₃	C ₅ H ₁₁ AsO ₂	C ₂ H ₇ AsO ₂
Chemical structure			
Identification numbers:			
CAS registry	98-50-0	64436-13-1	75-60-5
NIOSH RTECS ^b	CF7875000	CH9750000	CH7525000
EPA hazardous waste	D004	No data	U136/D004
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	No data	No data	UN1572/IMDG 6.1
HSDB	432	No data	360
EINECS	202-674-3	No data	200-883-4
NCI	No data	No data	No data

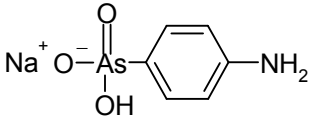
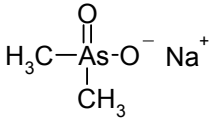
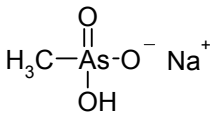
4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Chemical Identity of Selected Organic Arsenic Compounds^a

Characteristic	Disodium methane- arsonate	Methanearsonic acid	3-Nitro-4-hydroxy-phenyl- arsonic acid
Synonym(s)	DSMA; disodium monomethane arsonate	Arsonic acid, methyl-; monomethylarsonic acid	Roxarsone; 3-nitro- 4-hydroxyphenylarsonic acid; 3-Nitro-10
Registered trade name(s)	Ansar 8100; Arrhenal; Ansar DSMA Liquid; Dinate; Crab-E-Rad; Chipco Crab Kleen; Arsinyl; Sodar; Methar; Drexel DSMA Liquid; Di- Tac; Ansar 184; Weed-E- Rad; Versar DSMA-LQ; Calar-E-Rad; Dal-E-Rad; Jon-Trol; Namate	No data	No data
Chemical formula	CH ₃ AsO ₃ Na ₂	CH ₃ AsO ₃	C ₆ H ₆ AsNO ₆
Chemical structure			
Identification numbers:			
CAS registry	144-21-8	124-58-3	121-19-7
NIOSH RTECS ^b	PA2275000	PA1575000	CY5250000
EPA hazardous waste	D004	D004	D004
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	No data	No data	No data
HSDB	1701	845	4296
EINECS	205-620-7	204-705-6	204-453-7
NCI	No data	No data	C5608

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Chemical Identity of Selected Organic Arsenic Compounds^a

Characteristic	Sodium arsanilate	Sodium dimethylarsinate	Sodium methanearsonate
Synonym(s)	(4-Aminophenyl)arsonic acid sodium salt; arsanilic acid sodium salt; arsamin; atoxyl; soamin; trypoxyI	Sodium cacodylate; cacodylic acid, sodium salt; sodium dimethylarsonate	Arsonic acid, methyl-, monosodium salt; monosodium acid metharsonate; MSMA
Registered trade name(s)	No data	Ansar 160; Ansar 560; Bolle-Eye; Chemaid; Phytar 560, component of (with 012501); Rad-E-Cate 25.	Ansar 529; Ansar 170; Target MSMA; Phyban H.C.; Deconate; Mesamate; Bueno; Monate Merge 823; Dal-E-Rad; Weed-S-Rad; Arsanote liquid; Silvisar 550.
Chemical formula	C ₆ H ₇ AsNO ₃ Na	C ₂ H ₆ AsO ₂ Na	CH ₄ AsO ₃ Na
Chemical structure			
Identification numbers:			
CAS registry	127-85-5	124-65-2	2163-80-6
NIOSH RTECS ^b	CF9625000	CH7700000	PA2625000
EPA hazardous waste	D004	D004	D004
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	UN2473/IMDG 6.1	UN1688/IMDG 6.1	No data
HSDB	5189	731	754
EINECS	204-869-9	204-708-2	218-495-9
NCI	C61176	No data	C60071

^aAll information obtained from HSDB 2007 and CHEMIDplus 2007, except where noted.

^bRTECS 2007

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = Dept. of Transportation/United Nations/North America/Intergovernmental Maritime Dangerous Goods Code; EINECS = European Inventory of Existing Chemical Substances; 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 Chemical Substances

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-3. Physical and Chemical Properties of Arsenic and Selected Inorganic Arsenic Compounds^a

Property	Arsenic	Arsenic acid	Arsenic pentoxide	Arsenic trioxide
Molecular weight	74.9216	141.944	229.840	197.841
Color	Silver-gray or tin-white	White ^b	White	White
Physical state	Solid	Solid ^b	Solid	Solid
Melting point	817 °C (triple point)	35 °C	Decomposes at ~300 °C	313 °C (claudetite) 274 °C (arsenolite)
Boiling point	614 °C sublimes	Loses H ₂ O at 160 °C ^b	No data	460 °C
Density	5.778 g/cm ³ at 25 °C	~2.2 g/cm ³	4.32 g/cm ³	3.865 g/cm ³ (cubes) 4.15 g/cm ³ (rhombohedral crystals)
Odor	Odorless	No data	No data	Odorless
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	Insoluble	302 g/L at 12.5 °C ^b	2,300 g/L at 20 °C	17 g/L at 16 °C
Organic solvent(s)	No data	Soluble in alcohol, glycerol ^b	Soluble in alcohol	Practically insoluble in alcohol, chloroform, ether; soluble in glycerol
Other	Insoluble in caustic and nonoxidizing acids	No data	Soluble in acid, alkali	Soluble in dilute hydrochloric acid, alkali hydroxide, carbonate solution
Partition coefficients:				
Log K _{ow}	No data	No data	No data	No data
Log K _{oc}	No data	No data	No data	No data
pK _a	No data	pK _{a1} =2.22; pK _{a2} =6.98 pK _{a3} =11.53 ^c	No data	No data
Vapor pressure	7.5x10 ⁻³ mmHg at 280 °C	No data	No data	2.47x10 ⁻⁴ mmHg at 25 °C
Autoignition temperature	No data	No data	No data	Not flammable
Flashpoint	No data	No data	No data	No data
Flammability limits in air	No data	No data	No data	No data
Conversion factors	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-3. Physical and Chemical Properties of Arsenic and Selected Inorganic Arsenic Compounds^a

Property	Calcium arsenate	Gallium arsenide	Disodium arsenate	Sodium arsenite
Molecular weight	398.072	144.64	185.91	130.92
Color	Colorless	Dark gray	Colorless ^d	White to gray-white
Physical state	Solid	Solid	Solid ^d	Solid
Melting point	Decomposes on heating	1,238 °C	57 °C ^d	No data
Boiling point	No data	No data	No data	No data
Density	3.620 g/cm ³	5.3176 g/cm ³ at 25 °C	1.87 g/cm ^d	1.87 g/cm ³
Odor	Odorless	Garlic odor	Odorless ^d	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	0.13 g/L at 25 °C	<1 mg/mL at 20 °C	Soluble 1:3 parts in water ^d	Freely soluble in water
Organic solvents	Insoluble	<1 mg/mg dimethyl sulfoxide, ethanol, methanol, acetone	Slightly soluble in alcohol; soluble in glycerol ^d	Slightly soluble in alcohol
Other	Soluble in dilute acids	Soluble in hydrochloric acid	Slightly soluble in alkaline solution ^d	No data
Partition coefficients:				
Log K _{ow}	No data	No data	No data	No data
Log K _{oc}	No data	No data	No data	No data
pK _a	No data	No data		
Vapor pressure	~0 mmHg at 20 °C	No data	No data	No data
Autoignition temperature	Not combustible	No data	No data	Not combustible
Flashpoint	No data	No data	No data	No data
Flammability limits in air	No data	No data	No data	No data
Conversion factors	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

^aAll information from HSDB 2007, except where noted.^bValue for arsenic acid hemihydrate^cNRC 1999^dValue for disodium arsenate heptahydrate

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-4. Physical and Chemical Properties of Selected Organic Arsenic Compounds^a

Property	Arsenilic acid	Arsenobetaine	Dimethylarsinic acid
Molecular weight	217.06	196.1 ^b	138.00
Color	White	No data	Colorless
Physical state	Solid	Solid ^b	Solid
Melting point	232 °C	203–210 °C (decomposes) ^b	195 °C
Boiling point		No data	>200 °C
Density	1.9571 g/cm ³ at 10 °C	No data	No data
Odor	Practically odorless	No data	Odorless
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	Slightly soluble in cold water; soluble in hot water	No data	2,000 g/L at 25 °C
Organic solvent(s)	Slightly soluble in alcohol; soluble in amyl alcohol; insoluble in ether, acetone, benzene, chloroform	No data	Soluble in alcohol; insoluble in diethyl ether
Acids	Slightly soluble in acetic acid; soluble in alkali carbonates; moderately soluble in concentrated mineral acids; insoluble in dilute mineral acids	No data	Soluble in acetic acid
Partition coefficients:			
Log K _{ow}	No data	No data	No data
Log K _{oc}	No data	No data	No data
pK _a	No data	2.2 ^c	1.57
Vapor pressure	No data	No data	No data
Henry's law constant	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability	No data	No data	Nonflammable
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	No data

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-4. Physical and Chemical Properties of Selected Organic Arsenic Compounds^a

Property	Methanearsonic acid	3-Nitro-4-hydroxy-phenylarsonic acid	Sodium arsanilate
Molecular weight	139.97	263.03	239.04
Color	White	Pale yellow	White or creamy white
Physical state	Solid	Solid	Solid
Melting point	160.5 °C	No data	No data
Boiling point	No data	No data	No data
Density	No data	No data	No data
Odor	No data	No data	Odorless
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	256 g/L at 20 °C	Slightly soluble in cold water; soluble in about 30 parts boiling water	Soluble 1 part in 3 parts water
Organic solvents	Soluble in ethanol	Soluble in methanol, ethanol, acetone; insoluble in ether, ethyl acetate	Soluble 1 part in 150 parts alcohol; practically insoluble in chloroform, ether
Acids	No data	Soluble in acetic acid, alkalies; sparingly soluble in dilute mineral acids	No data
Partition coefficients:			
Log K _{ow}	No data	No data	No data
Log K _{oc}	No data	No data	No data
pK _a	pK _{a1} =4.1; pK _{a2} =9.02	No data	No data
Vapor pressure at 25 °C	<7.5x10 ⁻⁸ mmHg	No data	No data
Henry's law constant	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability	No data	No data	No data
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	No data

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-4. Physical and Chemical Properties of Selected Organic Arsenic Compounds^a

Property	Disodium methanearsonate	Sodium dimethylarsinate	Sodium methanearsonate
Molecular weight	183.93	159.98	161.95
Color	White	Colorless to light yellow	White
Physical state	Solid	Solid	Solid
Melting point	>355 °C	200 °C	130–140 °C
Boiling point	No data	No data	No data
Density	1.04 g/cm ³	>1 g/cm ³ at 20 °C	1.55 g/mL ^d
Odor	No data	Odorless	Odorless
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	432 g/L at 25 °C	200 g/L at 25 °C	580 g/L at 20 °C
Organic solvents	Soluble in methanol; practically insoluble in most organic solvents	No data	Insoluble in most organic solvents
Acids	No data	No data	No data
Partition coefficients:			
Log K _{ow}	<1	No data	-3.10
Log K _{oc}	No data	No data	No data
pK _a	pK _{a1} =4.1; pK _{a2} =8.94	6.29	pK _{a1} =4.1; pK _{a2} =9.02
Vapor pressure at 25 °C	10 ⁻⁷ mmHg	No data	7.8x10 ⁻⁸ mmHg
Henry's law constant	No data	No data	No data
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability	Nonflammable	No data	Nonflammable
Conversion factors	No data	No data	No data
Explosive limits	No data	No data	No data

^aAll information from HSDB 2007, except where noted.^bCannon et al. 1981 (arsenobetaine as monohydrate)^cTeräsahde et al. 1996^dValue for Ansar 6.6