

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of selenium and selenium compounds is presented in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Selenium is a non-metal element with atomic number 34 and an atomic mass of 78.96 (Lide 2000). Selenium belongs to Group 6 (Group VIA) of the periodic table, located between sulfur and tellurium, and resembles sulfur both in its various forms and in its compounds. The six stable isotopes of selenium are ^{74}Se , ^{76}Se , ^{77}Se , ^{78}Se , ^{80}Se , and ^{82}Se . These isotopes occur naturally with approximate abundances of 0.87, 9.02, 7.58, 23.52, 49.82, and 9.19%, respectively (Hoffmann and King 1997). Artificial radioactive isotopes of selenium have also been created by neutron activation. The gamma-emitting isotope ^{75}Se has been used in diagnostic applications of medicine (Hoffmann and King 1997). Selenium exists in several allotropic forms. Three are generally recognized, but as many as six have been claimed (Lide 2000). The stable form at ordinary room temperatures is the grey or hexagonal form with a melting point of 220.5 °C (Lide 2000). The other two important forms are red (monoclinic) with a melting point of 221 °C and amorphous selenium, which exists in black and red forms. Black amorphous selenium is vitreous and is formed by the rapid cooling of liquid selenium. Red amorphous selenium is colloidal and is formed in reduction reactions (Hoffmann and King 1997). Important selenium oxidation states are -2, 0, +4, and +6.

The chemical properties of selenium are similar to sulfur. Selenium combines with metals and many nonmetals directly or in aqueous solution. The selenides resemble sulfides in appearance, composition, and properties (Hoffmann and King 1997). Selenium may form halides by reacting vigorously with fluorine and chlorine, but the reactions with bromine and iodine are not as rapid. Selenium does not react directly with hydrogen fluoride or hydrogen chloride, but decomposes hydrogen iodide to liberate iodine and yield hydrogen selenide (Hoffmann and King 1997). Selenium reacts with oxygen to form a number of oxides, the most stable of which is selenium dioxide.

Information regarding the physical and chemical properties of selenium and selenium compounds is located in Table 4-2.

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

Characteristic	Selenium	Hydrogen selenide	Selenic acid	Selenious acid
Synonyms	Elemental selenium; selenium base; selenium dust; colloidal selenium; selenium homopolymer ^b ; selenium alloy	Dihydrogen selenide; hydrogen selenide [H ₂ Se]; selenium anhydride; selenium dihydride; selenium hydride; selane	Selenic acid, liquid ^{DOT,b}	Monohydrated selenium dioxide; selenous
Registered trade name(s)	C.I. 77805; VANDEX ^b			
Chemical formula	Se	H ₂ Se	H ₂ SeO ₄	H ₂ SeO ₃
Wisewesser line notation	SE	H2 SE	H2.SE-04	H2SE-03
Identification numbers:				
CAS	7782-49-2	7783-07-5	7783-08-6	7783-00-8
NIOSH RTECS	VS7700000	MX1050000	VS6575000	VS7175000
EPA hazardous waste	No data	No data	No data	U204 ^c
OHM/TADS	7216880	No data	No data	No data
DOT/UN/NA/IMCO shipping	UN 2658 ^b	UN 2202; Hydrogen selenide; anhydrous	UN 1905; IMCO 8.0	No data
HSDB	4493	548	675	6065
NCI	No data	No data	No data	No data

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

Characteristic	Sodium selenate	Potassium selenate	Sodium selenide	Sodium selenite
Synonyms	Disodium selenate	Selenic acid, dipotassium salt ^b	Disodium monoselenide ^b	Disodium selenite; disodium selenium trioxide; selenious acid disodium salt; sodium selenium oxide
Registered trade name(s)	P-40 ^b ; Sel-Tox SS02 and SS-20 ^c	No data	No data	
Chemical formula	Na ₂ SeO ₄ ^d	K ₂ SeO ₄	Na ₂ Se ^b	Na ₂ SeO ₃ ^d
Wisewesser line notation	NA2 SE-04 ^b	KA2 SE-04	NA2 SE	NAS SE-03
Identification numbers:				
CAS	13410-01-0	7790-59-2	1313-85-5 ^b	10102-18-8
NIOSH RTECS	No data	VS6600000	WE0350000 ^b	VS7350000
EPA hazardous waste	No data	No data	No data	No data
OHM/TADS	No data	No data	No data	7217299
DOT/UN/NA/IMCO shipping	No data	No data	No data	UN 2630 ^b
HSDB	No data	No data	No data	768
NCI	No data	No data	No data	No data

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

Characteristic	Selenium dioxide	Selenium trioxide	Selenocystine	Selenomethionine
Synonyms	Selenious anhydride; selenium oxide; selenium oxide [SeO ₂]; selenous acid anhydride	No data	Selenium cystine ^b ; 3,3-diselenodi-DL-alanine ^b ; seleno-DL-cystine ^b ; DL-selenocystine ^b	Methionine, seleno ^b ; 2-amino-4-(methylselenyl) butyric acid; 2-amino-4-(methylseleno)
Registered trade name(s)	No data	No data		
Chemical formula	SeO ₂	SeO ₃ ^e	C ₂ H ₄ NO ₂ (CH ₂)Se 2(CH ₂)C ₂ H ₄ NO ₂	(CH ₃)Se(CH ₂) ₂ C ₂ H ₄ NO ₂
Identification numbers:				
CAS	7446-08-04	13768-86-0 ^f	1464-43-3 ^b	1464-42-2
NIOSH RTECS	VS8575000	No data	AY6030000 ^b	ES100000
EPA hazardous waste	V204 ^c	No data	No data	No data
OHM/TADS	7800105	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	677	No data	No data	No data
NCI	No data	No data	No data	No data

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

Characteristic	Selenium sulfide	Selenium disulfide
Synonyms	Selenium monosulfide; selenium sulfide [SeS]; selensulfid (German); sulfur selenide (SSe)	Selenium disulphide; selenium sulfide ^b ; sulfur selenide
Registered trade name(s)	No data	Exsel; Selsun Blue; Selsum ^b ; Seleen
Chemical formula	SeS	SeS ₂ ^b
Wisewesser line notation	SE S	SE S ₂ ^b
Identification numbers:		
CAS	744-34-6	7488-56-4
NIOSH RTECS	VTO525000	VS8925000
EPA hazard waste	V205 ^b	V205
OHM/TADS	8400272	8400272
DOT/UN/NA/IMCO shipping	No data	UN 2657
HSDB	679	No data
NCI	NCI-C50033	No data

^aAll information obtained from HSDB 2001, except where noted

^bRTECS 2001

^cEPA 1980a, 1980b (40 CFR 261.33)

^dBudavari et al. 1996

^eLide 2000

^fChemIDplus 3003

CAS = Chemical Abstracts Service; 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 Chemical Substances

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Table 4-2. Physical and Chemical Properties of Selenium and Selenium Compounds^a

Property	Selenium	Hydrogen selenide	Selenic acid	Selenious acid
Molecular weight	78.96	80.98	144.97	128.97
Color/form	Red, grey, or black	Colorless ^b	White hexagonal prisms; hygroscopic ^b	White hygroscopic prisms ^b
Physical state	Solid	Gas	Solid	Solid
Melting point	221 °C (red); 220.5 °C (grey); 180 °C (black) ^b	-65.73 °C	58 °C	70 °C (decomposes) ^b
Boiling point	685 °C	-41.3 °C	260 °C	None, loses water upon heating
Density (g/cm ³)	4.39 (red); 4.81 (grey); 4.28 (black) ^b	2.12 (-42 °C)	2.9508 (15 °C)	3.004 (15 °C)
Odor	Unknown; upon combustion, smells like rotten horseradish	Disagreeable odor	No data	No data
Odor threshold:				
Water (mg/m ³)	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	Insoluble	377 mL/100 mL at 4 °C; 270 mL/100 mL at 22.5 °C; 0.73 mL/100 mL at 20 °C ^c	Very soluble in hot water	90 parts dissolve in 100 parts of water at 0 °C; 400 parts in 100 parts at 90 °C
Organic solvent(s)	Insoluble in alcohol, slightly soluble in carbon disulfide (2 mg/100 mL, room temperature), soluble in ether	Soluble in carbon disulfide, carbonyl chloride	Decomposes in alcohol ^b	Very soluble in alcohol
Partition coefficients:				
Log K _{ow}	No data	No data	No data	No data
Log K _{oc}	No data	No data	No data	No data
Vapor pressure	1 mmHg at 356 °C (grey)	1,330 mmHg at -30 °C; 3,420 mmHg at 0.2 °C; 9,120 mmHg at 30.8 °C	No data	2 mmHg at 15 °C; 4.5 mmHg at 33 °C; 7 mmHg at 40.3 °C
Henry's Law constant	Not applicable	No data	Not applicable	Not applicable
Autoignition temperature	No data	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Selenium and Selenium Compounds^a

Property	Selenium	Hydrogen selenide	Selenic acid	Selenious acid
Flashpoint	No data	Not applicable	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors	No data	ppm selenium to mg Selenium/m ³ in air (20 °C): ppm selenium x 3.23=mg selenium/m ³ to ppm selenium in air (20 °C): mg selenium/m ³ x 0.31=ppm selenium (v/v)	No data	No data
Explosive limits	Unknown ^d	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Selenium and Selenium Compounds^a

Property	Sodium selenate	Potassium selenate	Sodium selenide	Sodium selenite
Molecular weight	188.94	221.15	124.94	172.94
Color/form	White crystals	Colorless crystals or white powder	Crystalline; turns red on exposure to air and deliquesces	White tetragonal crystals ^b
Physical state	Solid	Solid	Solid	Solid
Melting point	No data	No data	>875 °C	No data
Boiling point	No data	No data	No data	No data
Density (g/cm ³)	1.61 ^b	3.07	2.625 (10 °C)	No data
Odor	No data	No data	No data	No data
Odor threshold: Water (mg/m ³)	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility: Water	Very soluble in water	Soluble in about 1 part of water	Decomposes in water	Freely soluble in water
Organic solvent(s)	No data	No data	No data	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
Vapor pressure	No data	No data	No data	No data
Henry's Law constant	No data	No data	No data	No data
Autoignition temperature	No data	No data	Not flammable ^e	Not flammable ^e
Flashpoint	No data	No data	Not flammable ^e	Not flammable ^e
Flammability limits	No data	No data	Not flammable ^e	Not flammable ^e
Conversion factors	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Selenium and Selenium Compounds^a

Property	Selenium dioxide	Selenium trioxide	Selenocystine	Selenomethionine
Molecular weight	110.96	126.96 ^b	334.12 ^c	196.11
Color/form	Lustrous, tetragonal needles; yellowish-green vapor	White crystals ^b	No data	Transparent, hexagonal sheets or plates; metallic luster or crystals
Physical state	Solid	Solid	No data	Solid
Melting point	340 °C; sublimes at 315 °C ^b	118 °C ^b	No data	DL form: 265 °C (decomposes); L form: 266–268 °C
Boiling point	None ^b	Sublimes ^b	No data	Not applicable
Density (g/cm ³)	3.954 (15 °C)	3.44 ^b	No data	No data
Odor	Pungent sour smell	No data	No data	No data
Odor threshold:				
Water (mg/m ³)	0.0002 ^e	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water (g/100 mL)	38.4 at 14 °C;	Soluble in water	No data	No data
Organic solvent(s) (parts/100 parts solvent)	in methanol: 10.16 at 11.8 °C; in 93% ethanol: 6.67 at 14 °C; in acetone: 4.35 at 15.3 °C; in acetic acid: 1.11 at 13.9 °C; soluble in benzene	No data	No data	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
Vapor pressure	12.5 mm Hg at 70 °C; 20.2 mm Hg at 94 °C; 39.0 mm Hg at 181 °C; 760 mm Hg at 315 °C; 848 mm Hg at 320 °C	No data	No data No data	No data No data
Henry's Law constant	Not applicable	Not applicable	No data	No data
Autoignition temperature	Not flammable ^e	Not flammable ^e	No data	No data
Flashpoint	Not flammable ^e	Not flammable ^e	No data	No data

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Table 4-2. Physical and Chemical Properties of Selenium and Selenium Compounds^a

Property	Selenium dioxide	Selenium trioxide	Selenocystine	Selenomethionine
Flammability limits	Not flammable ^e	Not flammable ^e	No data	No data
Conversion factors	ppm (v/v) to mg/m ³ in air (20 °C): ppm (v/v) x 4.53=mg/m ³ ; mg/m ³ to ppm (v/v) in air (20 °C): mg/m ³ x 0.22=ppm (v/v)	No data	No data	No data
Explosive limits	No data	No data	No data	No data

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Table 4-2. Physical and Chemical Properties of Selenium and Selenium Compounds^a

Property	Selenium sulfide	Selenium disulfide
Molecular weight	111.02 ^f	143.08 ^f
Color/form	Orange-yellow tablets or powder ^f	Bright red-yellow powder ^f
Physical state	Solid ^f	Solid ^f
Melting point	118–119 °C (decomposes) ^f	<100 °C ^f
Boiling point	No data	No data
Density (g/cm ³)	3.056 (0 °C) ^f	No data
Odor	No data	No data
Odor threshold:		
Water (mg/m ³)	No data	No data
Air	No data	No data
Solubility:		
Water	Insoluble	Insoluble
Organic solvent(s)	Insoluble in ether; decomposes in alcohol ^f	No data
Partition coefficients:		
Log K _{ow}	Not applicable	No data
Log K _{oc}	Not applicable	No data
Vapor pressure	Not applicable	Not applicable
Henry's Law constant	Not applicable	Not applicable
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	No data	No data
Conversion factors	No data	No data
Explosive limits	No data	No data

^aAll information obtained from Budavari et al. 1996, unless otherwise noted.

^bLide 2000

^cRTECS 2001

^dNIOSH/OSHA 1981

^eWeiss 1986

^fLide 1993

Note: The gray metallic form is the most stable form of selenium (Budavari et al. 1996).