

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of sulfur trioxide, sulfuric acid, and oleum (fuming sulfuric acid) is located in Table 3-1.

The acid strength of sulfuric acid is designated as percentage sulfuric acid or degrees Baume (°Bé) (IARC 1992). Degrees Baume is a mathematical relationship with specific gravity ($Bé = 145 - [145/\text{specific gravity}]$) that is consistent at concentrations below 93.2% sulfuric acid. At higher concentrations, the acid is referred to in terms of percentage sulfuric acid. The strength of oleum is indicated by the percentage of free dissolved sulfur trioxide, or as the equivalent percentage of 100% sulfuric acid.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of sulfur trioxide, sulfuric acid, and oleum (fuming sulfuric acid) is located in Table 3-2.

Table 3-1. Chemical Identity of Sulfur Trioxide, Sulfuric Acid, and Oleum

Characteristic	Sulfur trioxide	Sulfuric acid	Oleum	Reference
Synonyms	Sulfur trioxide; sulfur oxide; sulfuric anhydride; sulfan	Diothionic acid; brown oil; oil of vitriol; vitriol oleum; vitriol brown oil; dripping acid; BOV	Fuming sulfuric acid; disulphuric acid; dithionic acid; pyrosulphuric acid	HSDB 1998
Registered trade name(s)	Sulfan®	No data	No data	HSDB 1998
Chemical formula	SO ₃	H ₂ SO ₄	H ₂ SO ₄ with free SO ₃	HSDB 1998
Chemical structure				
Identification numbers:				
CAS registry	7446-11-9	7664-93-9	8014-95-7	HSDB 1998
NIOSH RTECS	WT4830000	WS5600000	WS5605000	HSDB 1998
EPA hazardous waste	No data	No data	No data	
OHM/TADS	No data	7216915	8500424	OHM/TADS98
DOT/UN/NA/IMCO shipping	UN1829, IMO 8.0 (inhibited), IMO 2.0 (uninhibited)	UN1830(≤65.25%), UN1832 (spent), UNI786 IMO 8.0	UN1831, IMO 8.0	HSDB 1998
HSDB	6338	1811	1236	HSDB 1998
NCI	No data	No data	No data	

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

Table 3-2. Physical and Chemical Properties of Sulfur Trioxide, Sulfuric Acid, and Oleum^a

Property	Sulfur trioxide	Sulfuric acid	Oleum	Reference
Molecular weight	80.06	98.07	178.14	HSDB 1998 Lide 1993
Color	Silky fiber needle (α); asbestos-like fiber (β); metastable	Colorless liq.	colorless or slightly colored	
Physical state	Gas, liquid, or solid	liquid	heavy, oily liquid	
Melting point	16.83°C (α); 62.4°C (β)	10.36°C (100%)	No data	
Boiling point	44.8°C (α); 50°C (β)(subl)	350 ± 0.5 (100%)	No data	
Density	-357 g/L at 0°C, 1.97 g/cm ³ at 20°C	1.841 (96-98%)	114.70 lb/ft ³	
Odor	No data	Odorless	No data	
Odor threshold:				
Water	No data	No data	No data	
Air	No data	Low: 1.0 mg/m ³ ; high: 1.0 mg/m ³ ; irritating: 1.10 mg/m ³	No data	
Solubility:				
Water at 0°C	No data	No data	No data	
Water at 20°C	No data	No data	No data	
Water at 25°C	No data	No data	No data	
Organic solvent(s)	No data	Decomp. Alcohol	No data	HSDB 1998
Partition coefficients:				
Log K _{ow} @ 25°C	No data	1.92	No data	
Log K _{oc}	No data	No data	No data	
Vapor pressure	73 mm Hg at 25°C (α); 344 mm Hg at 25°C (β)	1 mm Hg at 145.8°C	No data	HSDB 1998
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 limits	No data	Nonflammable	Nonflammable	
Conversion factors	1 ppm = 0.31 mg/m ³	1 ppm = 4.08 mg/m ³	No data	
Explosive limits	No data	No data	No data	HSDB 1998

^aLide, David. 1994. CRC Handbook of Chemistry and Physics. 74th ed. Boca Raton, FL: CRC Press.

