CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

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

Table 4-1. Chemical Identity of Thallium and Compounds[a]

Characteristic	Thallium	Thallium I acetate	Thallium III chloride	Thallium I nitrate
Synonym(s) and registered trade name(s)	Ramor[b]	Thallous acetate; thallium (1+) salt	Thallic chloride	Thallous nitrate; nitric acid, thallium (1+) salt
Chemical formula	Tl	$TlC_2H_3O_2$	$TlCl_3$	$TlNO_3$
SMILES	[Tl]	CC(=O)[O-].[Tl+]	[Tl](Cl)(Cl)Cl	[Tl+].[O-][N+](=O)[O-]
Chemical structure	Not applicable	Not applicable	Not applicable	Not applicable
CAS Registry Number	7440-28-0	563-68-8	13453-32-2	10102-45-1

Characteristic	Thallium III oxide	Thallium I sulfate	Thallium I carbonate
Synonym(s) and registered trade name(s)	Thallic oxide	Thallous sulfate	Thallous carbonate; carbonic acid; dithallium carbonate
Chemical formula	Tl_2O_3	Tl_2SO_4	Tl_2CO_3
SMILES	O=[Tl]O[Tl]=O	[Tl+].[Tl+].[O-]S([O-])(=O)=O	[Tl+].[Tl+].[O-]C([O-])=O
Chemical structure	Not applicable	Not applicable	Not applicable
CAS Registry Number	1314-32-5	7416-18-6	6533-73-9

Characteristic	Thallium I bromide	Thallium I iodide	Thallium I fluoride
Synonym(s) and registered trade name(s)	Thallium monobromide; thallous bromide	Thallous iodide	Thallium monofluoroide; thallous fluoride
Chemical formula	TlBr	TlI	TlF
SMILES	Br[Tl]	I[Tl]	F[Tl]
Chemical structure	Not applicable	Not applicable	Not applicable
CAS Registry Number	7789-40-0	7790-30-9	7789-27-7

[a]All information obtained from EPA (1998a), except where noted.
[b]NLM 2024

CAS = Chemical Abstracts Service; SMILES = simplified molecular-input line-entry system

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of thallium and thallium compounds is presented in Table 4-2. Thallium only possesses two stable isotopes: ^{203}Tl and Tl^{205} with natural abundances of 29.54 and 70.48%, respectively (Migaszewski and Gałuszka 2021). Thirty-five short-lived thallium radionuclides have been generated, including ^{204}Tl (half-life of 3.78 years), ^{202}Tl (half-life of 12.2 days), and ^{201}Tl (half-life of 73 hours) (Belzile and Chen 2017). Thallium occurs in two oxidation states: as the monovalent form (thallous, Tl^{+}) such as Tl_2O, Tl_2SO_4, or Tl_2S in strongly reducing conditions and as the trivalent form under oxidizing and alkaline conditions (thallic, Tl_3^{3+}) such as Tl_2O_3, $Tl(OH)_3$ and $TlCl_3$ (Migaszewski and Gałuszka 2021). The monovalent form is more stable and is the predominant chemical species in the environment. Pure thallium is scarce in nature because the surface of metallic thallium is readily oxidized.

Table 4-2. Physical and Chemical Properties of Thallium and Compounds[a]

Property	Thallium	Thallium I acetate	Thallium III chloride	Thallium I nitrate
Molecular weight	204.38	263.43	310.74	266.39
Color	Blush-white	White	White	White
Physical state	Metal	Solid	Solid	Solid
Melting point	303.5°C	131°C	25°C	205°C[b]
Boiling point	1,457±10°C	No data	Decomposes	430°C[b]
Density at 20°C	11.85	3.76 at 137°C	No data	5.5
Odor	Odorless[c]	Odorless[c]	No data	Odorless[c]
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Taste threshold	No data	No data	No data	No data
Solubility:				
Water	Insoluble	Very soluble	Very soluble	95.5 g/L
Organic solvent(s)	Soluble in nitric or sulfuric acid	Very soluble in alcohol; insoluble in acetone	Soluble in alcohol and ether	Insoluble in alcohol; soluble in acetone
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 at 1,000°C	10 mmHg[b]	No data	No data	No data
Henry's law constant	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Thallium and Compounds[a]

Property	Thallium III oxide	Thallium I sulfate	Thallium I carbonate
Molecular weight	456.76	504.82	468.78
Color	Colorless	Colorless	Colorless
Physical state	Solid	Solid	Solid
Melting point	717±5°C	632°C	273°C
Boiling point	-20 at 875°C	Decomposes[b]	No data
Density	9.65–10.19 at 21°C	6.77	7.11
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Taste threshold	No data	No data	No data
Solubility:			
Water	Insoluble	48.7 g/L	40.3 g/L at 15.5°C
Organic solvent(s)	Soluble in acids; insoluble in alkalis	No data	Insoluble in alcohol, ether, and acetone
Partition coefficients:			
Log K_{ow}	No data	No data	No data
Log K_{oc}	No data	No data	No data
Vapor pressure at 1,000°C	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 limits	No data	No data	No data
Conversion factors	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Thallium and Compounds[a]

Property	Thallium I bromide	Thallium I iodide	Thallium I fluoride
Molecular weight	284.29	331.29	223.38
Color	Yellowish-white	Yellow red (at 170°C)	Colorless
Physical state	Solid	Solid	Solid
Melting point	480°C	440°C[c]	327°C
Boiling point	815°C	824°C[c]	655°C
Density	7.56 at 17.3°C	7.29	8.23 at 4°C
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Taste threshold	No data	No data	No data
Solubility:			
Water	0.5 g/L at 25°C	0.006 g/L	786 g/L at 15°C
Organic solvent(s)	Soluble in alcohol, insoluble in acetone	Insoluble in alcohol, slightly soluble in nitric acid	Slightly soluble in alcohol
Partition coefficients:			
Log K_{ow}	No data	No data	No data
Log K_{oc}	No data	No data	No data
Vapor pressure at 1,000°C	10 mm Hg at 517°C[b]	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

[a]All information obtained from Lide (2005), except where noted.
[b]EPA 1988.
[c]NLM 2024.