

(14) Thionyl chloride, SOCl_2
CAS No. 7719-09-7
HS No. 28.12.10.90
TDG No. 1836
NIOSH/RTECS No. XM5150000
Merck 9278

Synonyms: Sulfinyl chloride, sulfur chloride oxide, sulfurous dichloride, sulfurous oxychloride, thionyl dichloride.

Physical properties: MW: 118.96, mp: -105°C , bp: 79°C , d.1.631, n_D^{20} 1.5190, a colourless to yellow-red liquid with a suffocating odour. Soluble in benzene, carbon tetrachloride and chloroform.

Synthesis: It is prepared by the reaction of sulphur dichloride with (1) sulphur trioxide, (2) sulphur dioxide and chloride, or (3) sulphuryl chloride (SO_2Cl_2) obtained from sulphur dioxide and chlorine. It can be prepared by a batch process but the major commercial process appears to be the continuous reaction of SO_2 (or SO_3) with SCl_2 (or S_2Cl_2) mixed with excess Cl_2 in the gas phase over activated carbon. Purification requires the removal of unchanged sulphur chlorides by forming adducts with e.g. styrene as the thionyl chloride is redistilled; commercial thionyl chloride is 98-99.6% pure.

Reactivity: It has a very significant organic chemistry with organic compounds having hydroxyl groups. Carboxylic acids are converted to acyl halides, alcohols to alkyl halides (or alkyl sulphites on chlorosulphites) amongst others. It is a powerful chlorinating agent.

Toxicology: It is toxic by inhalation, it fumes in moist air to produce SO_2 and HCl which are severe toxic hazards. It is a corrosive irritant to skin, eyes and mucous membranes. It reacts violently with ammonia, dimethylformamide, and dimethyl sulphoxide. Decomposition produces toxic fumes, its TLV is 1 ppm.

Uses: Its main use is the conversion of acids to acid chlorides for use as intermediates in the manufacture of pesticides, herbicides, surfactants, drugs, vitamins, dyestuffs and engineering thermoplastics. There is also a lithium-thionyl chloride high density battery.

Suppliers: There are nine suppliers listed: USA (2), PRC (1), India (1), Japan (2), UK (1), Spain (1) and Switzerland (1). SRI international lists two suppliers in the USA.