

Let's Take a PEEK at the PEAC Software

PEAC Example-Methyl Mercaptan

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PEAC Example – Methyl Mercaptan

This month our example is Methyl Mercaptan, which has a chemical formula of (CH₃SH). Methyl Mercaptan is listed under the UN # (United Nations Number) by the US Department of Transportation: UN 1064. Methyl Mercaptan is listed as CAS# (Chemical Abstract Service Number) 74-93-1.

Persons exposed only to Methyl Mercaptan pose little risk of secondary contamination to personnel outside the Hot Zone.

Methyl Mercaptan is a colorless flammable gas with unpleasant odor described as rotten cabbage. It is easily ignited. When heated to decomposition, it emits highly toxic fumes and flammable vapors. Vapors from liquified Methyl Mercaptan gas are heavier than air and may collect in low-lying areas. Olfactory fatigue may prevent adequate warning of hazardous concentrations.

Methyl Mercaptan is highly irritating when it contacts moist tissues such as the eyes, skin, and upper respiratory tract. It can also induce headache, dizziness, nausea, vomiting, coma, and death. Ingestion of Methyl Mercaptan is unlikely since it is a gas at ambient temperatures.

Uses: Methyl Mercaptan is produced by the reaction of hydrogen sulfide with methanol. It is used as a gas odorant; an intermediate in the production of pesticides, jet fuels, and plastics; in the synthesis of methionine; and as a catalyst.

Physical Properties:

Description: Colorless flammable gas at room temperature

Warning properties: Odor does not provide adequate warning of hazard

Molecular weight: 48.1 daltons

Boiling point: (760 mm Hg) = 43 °F (6 °C)

Freezing point: -186 °F (-123 °C)

Specific gravity (liquid): 0.87 at 0 °C

Vapor pressure: 1,520 mm Hg at 26 °C

Gas density: 1.66 (air = 1)

Water solubility: 23.3 g/L at 20 °C

Flammability: flammable limits 3.9% to 21.8% at room temperature

Synonyms include methanethiol, mercaptomethane, thiomethanol, methyl sulfhydrylate, and thiomethyl alcohol.

Incompatibilities: Methyl mercaptan is incompatible with strong oxidizers, bleaches, copper, aluminum, and nickel-copper alloys.

Description: At room temperature (above 43 °F), Methyl Mercaptan is a colorless gas with an unpleasant odor described as rotten cabbage. It is slightly soluble in water. It is generally shipped as a liquefied compressed gas. When heated to decomposition, it emits toxic fumes, such as sulfur dioxide, and flammable vapors. Methyl Mercaptan should be stored in cool, well-ventilated places. The main toxic effect of exposure to Methyl Mercaptan is irritation of the respiratory airway, skin, and eyes.

Standards and Guidelines

OSHA PEL (permissible exposure limit) = 10 ppm (20 mg/m³) NIOSH REL (recommended exposure limit) = 0.5 ppm

NIOSH IDLH (immediately dangerous to life or health) = 150 ppm

AIHA ERPG-2 (maximum airborne concentration below which it is believed that nearly all persons could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair their abilities to take protective action) = 25 ppm.

Routes of Exposure

Inhalation Inhalation is the major route of exposure to Methyl Mercaptan. An odor threshold of 0.002 ppm has been reported for Methyl Mercaptan, but olfactory fatigue may occur and thus, it **may not provide adequate warning of hazardous concentrations**. Vapors of liquified Methyl Mercaptan gas are heavier than air and spread along the ground. Exposure in poorly ventilated, enclosed, or low lying areas can result in asphyxiation because of respiratory paralysis.

Children exposed to the same levels of Methyl Mercaptan as adults may receive a larger dose because they have a greater lung surface area:body weight ratios and higher minute volume:weight ratios. In addition, they may be exposed to higher levels than adults in the same location because of their short stature and the higher levels of Methyl Mercaptan found nearer to the ground.

Skin/Eye Contact Direct contact with liquid Methyl Mercaptan or the gas may cause frostbite injury or irritation of the eyes and skin.

Ingestion Ingestion is unlikely to occur because Methyl Mercaptan is a gas at room temperature.

Health Effects

Methyl Mercaptan gas is irritating to the eyes, skin, and respiratory tract. Edema of the airway and lungs can occur. Other possible effects include headache, dizziness, tremors, and seizures, and nausea and vomiting, and lack of coordination. The gas is rapidly absorbed in the lungs. Skin and eye absorption are minimal; however, upon direct contact with eyes or skin, liquified Methyl Mercaptan will likely cause frostbite injury.

Methyl Mercaptan is a central nervous system depressant that acts on the respiratory center to produce death by respiratory paralysis.

Individuals with pre-existing respiratory, cardiac, nervous system, or liver impairment may be more susceptible to exposure to Methyl Mercaptan.

Acute Exposure Methyl Mercaptan inhibits mitochondrial respiration by interfering with cytochrome c oxidase. It also inhibits several enzyme systems such as carbonic anhydrase, beta-tyrosinase, and sodium⁺, potassium⁺ATPase. The enzyme inhibition appears to be related to a thiol-metal interference.

Children do not always respond to chemicals in the same way that adults do. Different protocols for managing their care may be needed.

Respiratory Acute inhalation exposure can irritate the mucous membranes of the respiratory tract. This may cause cough, dyspnea, a sensation of tightness of the chest, and subsequent cyanosis. Respiratory depression, apnea, and pulmonary edema were observed in animals.

Children may be more vulnerable to gas exposure because of relatively higher minute ventilation per kg and failure to evacuate an area promptly when exposed.

Hematologic Severe hemolytic anemia may occur in people with glucose-6-phosphate dehydrogenase deficiency.

Neurologic Restlessness, headache, staggering, and dizziness may develop; severe exposure may lead to convulsions and coma.

Dermal Frostbite injury can occur from contact with the liquified gas. Because of their relatively larger surface area:weight ratio, children are more vulnerable to toxicants that may affect the skin.

Ocular/Ophthalmic High concentrations of Methyl Mercaptan can cause eye irritation.

Gastrointestinal Although ingestion is unlikely, irritation of the mouth, throat, and esophagus are possible. Nausea and vomiting may occur even with inhalation exposure to the gas.

Potential Sequelae Methyl Mercaptan exposure may result in altered heme synthesis.

Chronic Exposure Dermatitis can occur with chronic exposure to Methyl Mercaptan.

Carcinogenicity Methyl Mercaptan has not been classified for carcinogenic effects.

Reproductive and Developmental Effects No information is available regarding reproductive or developmental effects of Methyl Mercaptan in experimental animals or humans. Methyl Mercaptan is not included in *Reproductive and Developmental Toxicants*, a 1991 report published by the U.S. General Accounting Office (GAO) that lists 30 chemicals of concern because of widely acknowledged reproductive and developmental consequences.

Using the PEAC tool

In using the PEAC application we access information for the chemical by first locating Methyl Mercaptan in the database. The following figures show the screens displayed for chemical properties, Figure 1 for the *PEAC-WMD for Windows* application and Figure 2-4 for the *PEAC-WMD for the Pocket PC* application.

PEAC-WMD

File Edit Tools Help

Select **Lookup By** chemical name

Lookup By: Chemical Name

Enter the first few characters of the name

Lookup: methyl me

Chemical Properties

Methyl Mercaptan

Methyl Mercaptophos

Methyl Mercapto...

From the information display under the **Chemical Properties** the user can immediately from the **Guide Name** and **NFPA 704 Hazard Classification information** see the material is flammable and very toxic.

Additional information is provided about specific flammability and toxicity.

Methyl Mercaptan

GUIDE 117 Gases - Toxic - Flammable (Extreme Hazard)
UN 1064

Colorless gas; strong disagreeable odor

Formula: CH₃SH

Shipped as liquefied gas under its own vapor pressure. If heat or rupture, will rocket.

NFPA Information
Health: 4 Deadly
Fire: 4 Flash Point < 73°
Reactivity: 0 Stable

CAS NO: 74-93-1
Flash Point: 0°F
Lower Explosive Limit: 3.9%
Upper Explosive Limit: 21.8%
Boiling Point: 43°F
Melting Point: -186°F
Rel Vapor Density @68°F: 1.7
Vapor Pressure @68°F: 1.7 atm
Liquid Specific Gravity: 0.9
Ionization Potential: 9.44 eV
Yield Factor: 0.03
Molecular Weight: 48
IDLH: 150 ppm
TWA: 0.5 ppm
ERPG1: 0.005 ppm
ERPG2: 25 ppm
ERPG3: 100 ppm
TEEL1: 3 mg/m³
TEEL2: 50 mg/m³
TEEL3: 200 mg/m³

Methyl Parathion solid

Methyl pentane

Methyl Pentane

Methyl phenol

Methyl Phenyl Ether

Methyl phosphate

Methyl phosphite

Methyl phosphite ((MeO)3P)

Methyl phosphonate ((MeO)2HPO)

Methyl Phosphonic Acid

Methyl phosphonic acid, dimethyl ester

Methyl phosphonic dichloride

Methyl Phosphonic Dichloride

Methyl phosphonothioic dichloride

Methyl phosphonous acid, 2-(Bis[1-methylethyl] amino) ethyl ethyl e...

Methyl Phosphonous Dichloride

Methyl phthalate

Methyl Picric Acid

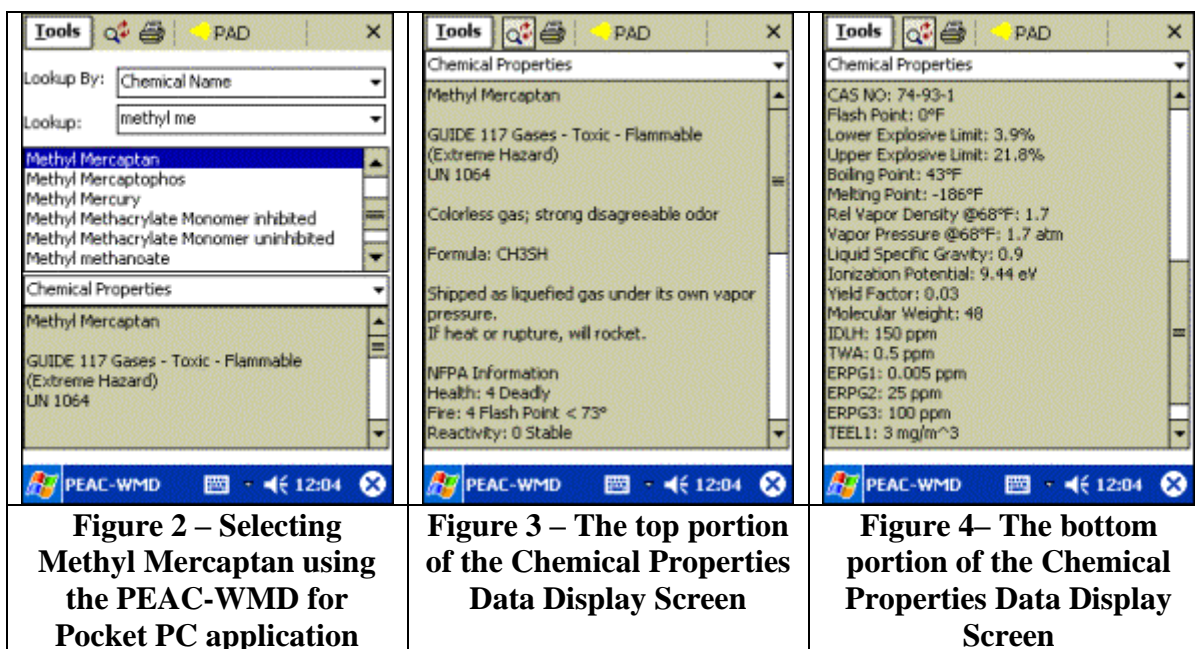
Methyl propenoate

Methyl Propionate

Methyl Mercaptan

Figure 1 - Using the Lookup By: Name for Methyl Mercaptan using the PEAC-WMD for Windows application

Review of the information displayed in the chemical properties screen whether in Figure 1 (above) or Figures 2-4 (below), show chemical properties values discussed earlier at the top of this discussion. As you can see below, the published toxicity values, e.g., IDLH, ERPGs, and the TEELs (Temporary Emergency Exposure Limits) published by Department of Energy are provided. We will use the IDLH as the Level of Concern when we develop the Protective Action Distance (PAD) a little later.



A benefit of using the PEAC tool is assistance in the development of an evacuation zone for those chemicals that produce a toxic vapor cloud. As with most of our examples, AristaTek creates a scenario for a spill or release of the specific chemical, and then we work through the development of a PAD (Protective Action Distance) to demonstrate how the PEAC system works.

For our hypothetical scenario using Methyl Mercaptan as the involved chemical we'll set the location to be natural gas processing facility located outside Houston, TX. The date is May 13, 2004, at midnight with a temperature of 65°F, wind speed of 2 mph and a clear sky. The hypothetical release involves a portable tank that contains Methyl Mercaptan and a ½" transfer line from the tank has been severed and can't be isolated. Vapor is flowing from the tank through the ½" line. The PEAC tool can provide guidance with regards to toxic vapor cloud that is released.

If you decide to follow along as we proceed through these examples, remember to set the location to Houston and set the date and time to the proper values, otherwise you'll compute different values. We'll use a terrain type of urban/forest since this is a manufacturing facility and has buildings and processing equipment in the immediate area.

As seen at the top of the data display screens, there is a yellow icon displayed; this is the PEAC icon for notifying the user that a Protective Action Distance can be calculated. Clicking or tapping on the PAD icon will display a screen as shown in Figure 5. Following through the screens, we provide information on the Meteorology, Container Size, and Type of Release (Source). The following figures demonstrate how we would work through our scenario to see what our Protective Action Distance should be.

<p>Meteorology</p> <p>It's midnight Houston in May and the temperature about 65°, wind is set for 2 mph, clear skies and the terrain is Urban/Forest since it's a processing facility setting.</p>	<p>Container</p> <p>We have selected from our list of container sizes the Portable Tank selection. This gets us a quick estimate of how much material might be involved.</p>	<p>Source</p> <p>We have selected a Hole or Pipe Release, and set the hole size to 0.5”.</p>

Figure 5 – Calculating a PAD using the PEAC-WMD System for May 13th

By pressing the right arrow at the top of the screen, the PEAC system will display a screen as shown in Figure 6. This calculates a **PAD** (Protective Action Distance) based on the default **Level of Concern** the IDLH of 150 ppm. This evacuation or standoff distance is based on the toxicity of Methyl Mercaptan, not the flammability.

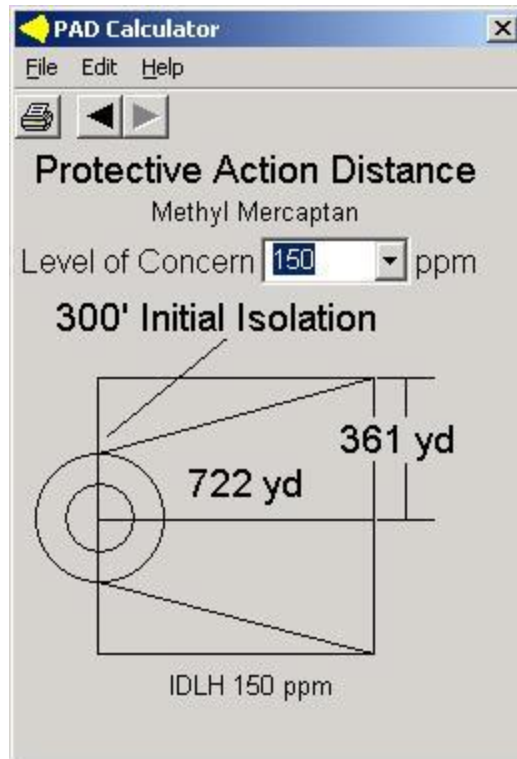


Figure 6 – Default PAD for Methyl Mercaptan using the IDLH of 150 ppm

If we want to calculate a PAD based on a toxicity level other than the IDLH, we can enter a value in the field for **Level of Concern** or we can select a value from our list of toxicity values shown in Figure 7. In this figure we select the ERPG-2 value or 25 ppm.

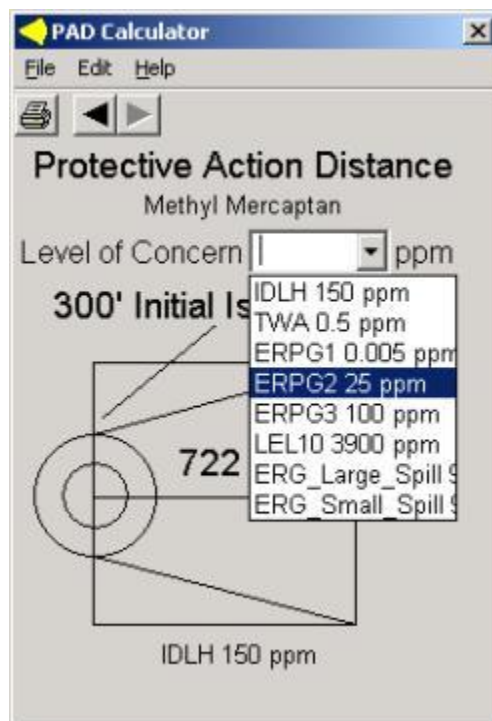


Figure 7 – Selecting another Level of Concern
The calculated PAD will be displayed, see Figure 8.



Figure 8 – Calculated PAD using the ERPG-2 Level of Concern

In addition to the toxicity of the released material, the user should also remember the flammability issue with Methyl Mercaptan and eliminate all ignition sources. At either the IDLH concentration of 150 ppm, or the ERPG-2 concentration of 25 ppm, there will be many complaints about the odor.

Substantial portions of this discussion were adapted from the Agency for Toxic Substances and Disease Registry (ATSDR) Web site for Medical Management Guidelines at: <http://www.atsdr.cdc.gov/>.