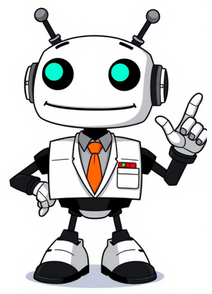
Click to verify



Please enable Javascript in order to use PubChem website. Diphenyl ketone [119-61-9], benzophenone, C6H5COC6H5, C13H10O, Mr 182.22. The stable form of diphenyl ketone consists of colorless rhombic prismatic crystals. Several unstable forms with lower melting points also exist. Diphenyl ketone is insoluble in water and readily soluble in organic solvents. Diphenyl ketone and substituted diphenyl ketones in particular are used mainly as photoinitiators for UV-curable printing inks and coatings. Diphenyl ketone is also used as an intermediate for pharmaceuticals and agricultural chemicals. It is employed in the perfume industry as a fixative and as a fragrance with a flowery note. Shiny white prismatic crystals with a sweet taste, smell like a rose, melting point is 47-49 , boiling point is 306 , insoluble in water, soluble in alcohol, ether and chloroform. Sunscreen cosmetics is the hot new products of cosmetics, almost all sunscreens contain benzophenone compound on the current market. Benzophenone compounds that protect the skin from harm, often is used to produce high product. In recent years, the cosmetics consumption of benzophenone grows continuesly. Recent studies suggest that fluorescence is also a harmful ultraviolet light source, so benzophenone expands the range of applications in the field of cosmetics, it has been extended to hair conditioners, lotions and lipsticks. In addition, the perfume fixative agent also can give spice sweet flavor, is used in many perfumes and soap flavor. Banana Boat company has developed a UVA ultraviolet-absorbing technology called AvoTriplex, which is benzophenone-based, adding a stabilizer to prevent the benzophenone from breaking down in the sun. Enhancer is also added into the formula, and stabilizer may act synergistically, to optimize benzophenone sunscreen capacity. Benzophenone Mainly used for the preparation of vanilla, butter and other flavorIt can be used as a fixative agent. Its weak sweet bay leaves fragrant , can be widely used in low-grade flavors, such as roses, bay leaves, sweet curd, shy flower, lily of the valley, sunflower, orchid, hawthorn flowers, incense and Wei Oriental flavor and other flavors. It is also used as an antioxidant in soaps, and occasionally used for almonds, berries, fruit, butter, nuts, peaches, vanilla beans and other food flavors in trace amount. Uses for photosensitive resins, coatings and adhesives. Benzophenone is an intermediate of UV absorbers, organic pigments, pharmaceuticals, perfume, insecticide . It is used for the production of bicyclic Piperidine Benztropine hydrobromide, diphenhydramine hydrochloride in the pharmaceutical industry . The product itself is a styrene polymerization inhibitor and a perfume fixative. Giving sweet taste to flavors, it is used in many perfumes and soap flavors. It is commonly used in soap flavor, used in ultraviolet absorbers, pigments, pharmaceuticals and reagents production, and also is low temperature fast curing agent for fluorine rubber. It serves to manufacturers to package the product in clear glass or plastic. Benzophenone is widely employed as a photo initiator in UV-curing applications such as inks, imaging and clear coatings in the printing industry. It acts as a UV blocker to prevent photo-degradation of the packaging polymers or its contents. It is light initiator for UV products, pharmaceutical intermediates, fragrances, light stabilizers etc. It is light pigment, medicine, perfume, pesticides intermediates, it can also be used for UV-curable resins, inks and coatings initiator. Benzophenone is widely used in the synthesis experiment as an indicator, it can be used as a indicator while handling toluene, benzene, THF, acetonitrile ect.; if there is a beautiful blue after added, it can be distillated and used, it is the best to kept in sodium, but the reason of generating blue is still a puzzle. Here is the reason from a foreign book about reactions mechanism : a radical anion generated by the one called carbonyl radical, benzophenone acts as the indicator is that benzophenone oxygen atoms in sodium capture electrons to generate dark blue carbonyl radical; the radicals perspective on the electrical aspect is stable, mainly used to indicate 'anaerobic conditions',Widely used. After the addition of benzophenone, more blue of the solution, indicating less oxygen in the solution, indirectly instructing the little water. However, whether the solution turns blue, is related to the added amount of benzophenone and processing solvent, THF (300ml) contains lots of water, and needs more than about 6 hours to reflux, and of course, it is related to the amount of processing solvent, the more the longer, toluene , benzene and other samples containing less aqueous need less reflux time, it is best to add the common desiccants to pretreat, such as: potassium carbonate, sodium sulfate, sodium hydroxide, etc., so that the processing time will be shortened. GRAS(FEMA)LD502897mg/kg(Mice, orally) There are different methods for synthesizing benzophenone. One method involves condensing benzyl chloride and benzene, followed by oxidation with nitric acid. Another method involves condensing benzene and carbon tetrachloride, followed by hydrolysis. In laboratory production, benzophenone is typically synthesized using aluminum chloride as a catalyst, with benzene reacting with benzoyl chloride. The final method involves condensing benzene and benzoyl chloride in the presence of aluminum chloride, followed by crystallization from ethanol. Benzophenone is a combustible, white,crystalline solid with a rose-like odor. Molecularweight=182.23; Specific gravity (H2O:1) = 1.085 at 50;Boiling point = 305; Freezing/Melting point = 48.5;Latent heat of vaporization=2.93 3 105 J/kg; Heat ofcombustion= -358 3 105 J/kg. Hazard Identification(based on NFPA-704 M Rating System): Health 1,Flammability 1, Reactivity 0. Insoluble in water. Benzophenone is a combustible, white, crystalline solid with a rose-like odor. soluble in ethanol, ether, chloroform and other organic solvents and monomers, insoluble in water. It is a free radical photoinitiator, mainly used in free radical UV curing systems, such as coatings, inks, adhesives, etc. It can be prepared in several ways, for example, by FriedelCrafts reaction of benzene and benzoyl chloride with aluminum chloride, or of benzene and carbon tetrachloride, and oxidation of diphenylmethane. Benzophenone has been found in various fruits, including Vitis vinifera L., black tea, cherimoya (Annona cherimola), mountain papaya (Carica pubescens), and soursop (Annona muricata L.). Benzophenone is used as a synthetic intermediatefor manufacture of pharmaceuticals and agricultural chemicals.It is also used as a photoinitiator in UV-curable printinginks, as a fragrance in perfumes, as a flavor enhancerin foods. Benzophenone can be added as aUV-absorbing agent to plastics, lacquers, and coatings at concentrationsof 28%. Benzophenone is commercially synthesized by the atmosphericoxidation of diphenylmethane using a catalyst ofcopper naphthenate. Alternatively, it can be produced by aFriedelCrafts acylation of benzene using either benzoylchloride or phosgene in the presence of aluminum chloride. ChEBI: Benzophenone is the simplest member of the class of benzophenones, being formaldehyde in which both hydrogens are replaced by phenyl groups. It has a role as a photosensitizing agent and a plant metabolite. Tetrahedron Letters, 36, p. 2285, 1995 DOI: 10.1016/0040-4039(95)00191-EChemical and Pharmaceutical Bulletin, 34, p. 3595, 1986 DOI: 10.1248/cpb.34.3595 Benzophenone(119-61-9) appears as white solid with a flowery odor. May float or sink in water. It is a widely used building block in organic chemistry, being the parent diarylketone. Insoluble in water. Ketones, such as Benzophenone, are reactive with many acids and bases liberating heat and flammable gases (e.g., H2). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H2) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO3, HNO3 + H2O2, and HClO4. Benzophenone can react with oxidizing materials. Ingestion causes gastrointestinal disturbances. Contact causes eye irritation and, if prolonged, irritation of skin. Flash point data for Benzophenone are not available, but Benzophenone is probably combustible. reagent type: reductant Unsubstituted benzophenone is largely used in chemicalapplications. It acts as a marker for photoallergy toketoprofen. Moderately toxic by ingestion andintraperitoneal routes. Combustible when heated.Incompatible with oxidizers. When heated todecomposition it emits acrid and irritating fumes. Benzophenone is used in UV curingof inks and coatings; as an intermediate; as an odor fixativein fragrances, flavoring, soaps; in the manufacture of pharmaceuticalsand insecticides; in organic syntheses. If this chemical gets into the eyes, remove anycontact lenses at once and irrigate immediately for at least15 min, occasionally lifting upper and lower lids. Seekmedical attention immediately. If this chemical contactsthe skin, remove contaminated clothing and wash immediately with soap and water. Seek medical attention immediately. If this chemical has been inhaled, remove fromexposure, begin rescue breathing (using universal precautions, including resuscitation mask) if breathing hasstopped and CPR if heart action has stopped. Transferpromptly to a medical facility. When this chemical hasbeen swallowed, rinse mouth and get medical attention. Lifetime dermal carcinogenicitystudies in mice and rabbits did not show any tumor excessin the treated animals. Female Swiss mice andNew Zealand White rabbits of both sexes were treated dermallywith 0, 5, 25, or 50% of benzophenone (0.02 mL) twicea week for 120 or 180 weeks. Weekly examination of therabbits did not reveal any reduction in survival or appearanceof tumors. Mice treated with benzophenone did not show anyexcess in the number of tumor-bearing animals or in totalnumber of tumors compared to untreated control animals.Although three skin tumors were observed in the benzophenone-treated mice (one case of squamous cell carcinoma andtwo cases of squamous cell papilloma), there were also threetumors (one carcinoma and toe papillomas) observed in thecontrol animals. Benzophenone's main metabolic pathway in the rabbit is by reduction to benzhydrol, which is excreted conjugated with glucuronic acid(Williams, 1959). Insoluble in water and glycerin, slightly soluble in Propylene glycol, 6% soluble in alcohol, soluble inmost perfume oils. Color CodeGreen: General storage may be used.Store in a cool, well-ventilated area away from sources ofignition and incompatible materials. UN1224 Ketones, liquid, n.o.s., Hazard Class: 3;Labels: 3Flammable liquid, Technical Name Required.UN3077 Environmentally hazardous substances, solid, n.o.s.,Hazard class: 9; Labels: 9Miscellaneous hazardous material,Technical Name Required. Crystallise it from MeOH, EtOH, cyclohexane, *benzene or pet ether, then dry in a current of warm air and store it over BaO or P2O5. It is also purified by zone melting and by sublimation [Itoh J Phys Chem 89 3949 1985, Naguib et al. J Am Chem Soc 108 128 1986, Gorman & Rodgers J Am Chem Soc 108 5074 1986, Ohamoto & Teranishi J Am Chem Soc 108 6378 1986, Naguib et al. J Phys Chem 91 3033 1987]. [Beilstein 7 III 2048, 7 IV 1357.] Oxidizing materials, such as dichromatesand permanganates. The initial threshold screening level (ITSL) for benzophenone is 100 g/m3 with an annual averaging time. AddtoMyChemicals PrintFriendlyPage Chemical Datasheet ChemicalIdentifiers | Hazards | ResponseRecommendations |PhysicalProperties |RegulatoryInformation | AlternateChemicalNames CAS Number UN/NA Number DOT Hazard Label USCG CHRIS Code BZP NIOSH Pocket Guide International Chem Safety Card none BENZOPHENONE NFPA 704data unavailable General Description White solid with a flowery odor. May float or sink in water. (USCG, 1999) Reactivity Alertsnone Air & Water Reactions Insoluble in water. Fire Hazard Flash point data for this chemical are not available, but it is probably combustible. (NTP, 1992) Health Hazard Ingestion causes gastrointestinal disturbances. Contact causes eye irritation and, if prolonged, irritation of skin. (USCG, 1999) Reactivity Profile Ketones, such as BENZOPHENONE, are reactive with many acids and bases liberating heat and flammable gases (e.g., H2). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H2) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO3, HNO3 + H2O2, and HClO4. This compound can react with oxidizing materials. (NTP, 1992) Belongs to the Following Reactive Group(s) Hydrocarbons, Aromatic Ketones Potentially Incompatible Absorbents No information available. Isolation and Evacuation Excerpt from ERG Guide 127 [Flammable Liquids (Water-Miscible)]: IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area for at least 50 meters (150 feet) in all directions. LARGE SPILL: Consider initial downwind evacuation for at least 300 meters (1000 feet).FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024) Firefighting Fire Extinguishing Agents Not to Be Used: Water may be ineffective.Fire Extinguishing Agents: Foam, dry chemical, carbon dioxide, water spray. (USCG, 1999) Non-Fire Response SMALL SPILLS AND LEAKAGE: Should a spill occur while you are handling this chemical, you should dampen the solid spill material with alcohol, then transfer the dampened material to a suitable container. Use absorbent paper dampened with alcohol to pick up any remaining material. Seal the absorbent paper, and any of your clothes, which may be contaminated, in a vapor-tight plastic bag for eventual disposal. Solvent wash all contaminated surfaces with alcohol followed by washing with a strong soap and water solution. Do not reenter the contaminate area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.STORAGE PRECAUTIONS: You should store this material in a refrigerator. (NTP, 1992) Protective Clothing Dust/mist respirator; goggles or face shield; rubber gloves (USCG, 1999) DuPont Tychem Suit Fabrics No information available. First Aid EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop. SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment. INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992) What is this information? The Physical Property fields include properties such as vapor pressure and boiling point, as well as explosive limits and toxic exposure thresholds The information in CAMEO Chemicals comes from a variety of data sources. Note: For Vapor Density and Specific Gravity, comparing the value to 1.0 can tell you if the chemical will likely sink/rise in air or sink/float in fresh water (respectively). Short phrases have been added to those values below as an aid. However, make sure to also consider the circumstances of a release. The Vapor Density comparisons are only valid when the gas escaping is at the same temperature as the surrounding air itself. If the chemical is escaping from a container where it was pressurized or refrigerated, it may first escape and behave as a heavy gas and sink in the air (even if it has a Vapor Density value less than 1). Also, the Specific Gravity comparisons are for fresh water (density 1.0 g/mL). If your spill is in salt water (density about 1.027 g/mL), you need to adjust the point of comparison. There are some chemicals that will sink in fresh water and float in salt water.Chemical Formula: Flash Point: greater than 270F (USCG, 1999) Lower Explosive Limit (LEL): data unavailable Upper Explosive Limit (UEL): data unavailable Autoignition Temperature: data unavailable Melting Point: alpha-118.6F; beta-79F; gamma-117F. (NTP, 1992) Vapor Pressure: data unavailable Vapor Density (Relative to Air): data unavailable Specific Gravity: 1.085 at 122F (USCG, 1999) - Denser than water; will sink Boiling Point: 582.6F at 760 mmHg (NTP, 1992) Molecular Weight: 182.21 (NTP, 1992) Water Solubility: Insoluble (