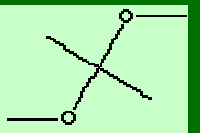
2,2-DIMETHOXYPROPANE



PRODUCT IDENTIFICATION	
CAS NO.	77-76-9
EINECS NO.	201-056-0
FORMULA	$(CH_3)_2C(OCH_3)_2$
MOL WT.	104.15
H.S. CODE	2911.00.5000
TOXICITY	
SYNONYMS	Acetone dimethyl acetal; Acetone dimethyl ketal; 2,2-Dimethoxypropane;
SMILES	C(OC)(OC)(C)C
CLASSIFICATION	
EXTRA NOTES	Dehydrating agent in electron microscopy specimen preparation.

PHYSICAL AND CHEMICAL PROPERTIES	
PHYSICAL STATE	clear liquid
MELTING POINT	-47 C
BOILING POINT	83 C
SPECIFIC GRAVITY	0.85
SOLUBILITY IN WATER	18 g/100g at 25 C
SOLVENT SOLUBILITY	Soluble in acetone, benzene, CCl
pH	
VAPOR DENSITY	
log P	1.38 (Octanol-water)
VAPOR PRESSURE	(mmHg at 25 C)
HENRY LAW CONSTANT	8.91E-05 (atm-m3/mole at 25 C)
OH RATE CONSTANT	3.92E-12 (cm3/molecule-sec at 25 C Atmospheric)
AUTOIGNITION	
NFPA RATINGS	
REFRACTIVE INDEX	1.376 - 1.378
FLASH POINT	-5 C
STABILITY	Stable under ordinary conditions.

EXTERNAL LINKS & GENERAL DESCRIPTION

Local: Acetals are geminal-diether derivatives of aldehyde by combination of an aldehyde molecule with two alcohol molecules and elimination of water. The formula is $RCH(OR')_2$, where R and R' are aliphatic or aromatic radicals. If the formula is $RCR'(OR'')_2$, it is called ketal derived by a combination of a ketone with two alcohols. The "acetal" also refer to independent structural units in certain biological and commercial polymers. Lower acetals are colorless volatile liquid used as a solvent and in cosmetics but higher acetals are solid. It is soluble in ether and alcohol but slightly soluble in water. It is unstable in acid but stable in base.

Acetal polymers (polyacetals) are tough and hard plastics used as substitutes for metals. Acetalhomopolymers are produced by the polymerization of formaldehyde. Acetal copolymers are produced are by the polymerization of formaldehyde with trioxane. In nature the most stable glucose exists as a cyclic hemiacetal and maltose is an acetal made from two glucose units.

Acetal formation is reversible (hydrolyzed back to their starting components by treatment with

aqueous acid). In order to achieve effective acetal formation an acid catalyst must be used and the water produced with the acetal must be removed. p-Toluene sulfonic acid is often used as a catalyst in the formation of acetal which water must be removed from the reaction mixture to escape reversible reaction. Water is removed azeotropically by distilation. (Toluene is the solvent). A way to remove water is to use an orthoester as a source of alcohol; water produced along with the acetal product is used up in hydrolysing the orthoester and producing more alcohol to be used in the reaction. Orthoester is a functional group which has three alkoxy groups attached to one carbon atom.

The importance of acetals as carbonyl derivatives lies chiefly in protecting groups for carbonyl groups in organic synthesis as they exhibit stability and lack of reactivity in neutral to strongly basic environments. Acylals, with the general formula $R\text{-}C(OOCR)_2$, is an another carbonyl protecting group. It is obtained by the reaction of aldehydes with acetic anhydride. Acetal molecules are used as an intermediate for the production of polymers, vitamins, carotenoid pigments, dyes, pharmaceuticals, pesticides, corrosion inhibitors, fragrances and perfumes.

Applications of 2,2-Dimethoxypropane:

- Preparation of 1,2-diols as acetonides
- Protection of 1,3-diols by acetonide formation.
- Protection of vic-diols via isopropylidenation.
- Interconversion of Carboxylic acid to ester
- Derivatization of Ketone to acetal using acid-catalyzed exchange of methoxy groups.
- Derivatization of fatty acids to fatty acid methyl esters

SALES SPECIFICATION	
APPEARANCE	clear liquid
ASSAY	99.0% min
WATER	0.2% max
TRANSPORTATION	
PACKING	50kgs in drum
HAZARD CLASS	3 (Packing Group: II)
UN NO.	1993
SAFETY INFORMATION	
Hazard Symbols: F XI, Risk Phrases: 11-36/37/38, Safety Phrases: 16-26-37/39	