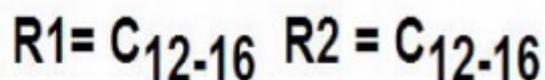
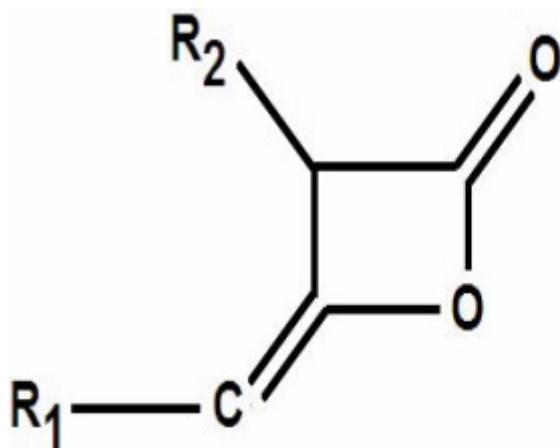


## Alkyl Ketene Dimer

### SYNONYMS

2-Oxetanone, 3-C14-16-alkyl 4-C15-17-alkylidene derivatives  
2-Oxetanone, 3-C12-16-alkyl 4-C13-17-alkylidene derivatives

### CHEMICAL STRUCTURE



### CHEMICAL FORMULA

$C_{30}H_{56}O_2$  to  $C_{37}H_{70}O_2$  (CAS No 98246-87-8)

$C_{28}H_{52}O_2$  to  $C_{36}H_{68}O_2$  (CAS No. 84989-41-3)

### IDENTIFIER DETAILS

CAS Number	:	98246-87-8 (structurally related compound 84989-41-3)
CoE Number	:	-
FEMA	:	-
EINECS Number	:	308-760-8
E Number	:	-

### SPECIFICATIONS

Melting Point: 43.6-56.4 °C

Boiling point: Decomposes above 200°C without boiling

## STATUS IN FOOD AND DRUG LAWS

### CoE limits:

Beverages (mg/kg)	Food (mg/kg)	Exceptions (mg/kg)
-	-	-

### Acceptable Daily Intake:

ADI (mg/kg)	ADI Set by	Date Set	Comments
-	-	-	-

### FDA Status: [CFR21]

Section Number	Comments
176.120	Indirect food additives for paper and board

## HUMAN EXPOSURE

**Natural occurrence:** Not reported to be found in nature.

**Reported Uses:** Alkyl Ketene di mer is predominantly used in the paper industry as a sizing agent in alkali paper making [Karademir 2002].

## TOXICITY DATA

Alkyl ketene di mers (AKDs) are waxy materials that are insoluble in water. Commercially they are prepared from the natural fatty acid sources such as stearic acid. The variation in chain lengths reflect the fact that the starting material may also vary in chain length. It is believed in general that AKD reacts with cellulose to form a beta keto-ester bond making the paper hydrophobic. AKD also reacts with water to form an unstable beta-keto acid which is unstable and then de-carboxylates to form a ketone. The reaction with rate between AKD and water is faster than that of AKD with cellulose fibre. The reaction between AKD and cellulose is believed by some to be key to water repellence and by others believe that this reaction does not take place and is not responsible for sizing [Karademir 2002].

Species	Test Type	Route	Reported Dosage
Rat	LD <sub>50</sub>	Oral	>10000 mg/kg
Rat	LD <sub>50</sub>	Oral	>2000 mg/kg
Rat	LD <sub>50</sub>	Oral	560 mg/kg
Rat	LD <sub>50</sub>	Inhalation	No deaths*
Rabbit	LD <sub>50</sub>	Dermal	6730 mg/kg
Mouse	LD <sub>50</sub>	Intraperitoneal	6800 mg/kg

[ESIS, 2009]

\* No deaths occurred at 20°C or saturated vapours for 12 rats exposed for 8 hours duration.

### Dermal toxicity

Dermal application of AKD, applied as a 40% aqueous dispersion was not irritating to the rabbit. AKD was not irritating when applied to the eye of rabbits [ESIS, 2009].

In the Buehler test a 20 % aqueous dispersion was non-irritating in the guinea pig [ESIS, 2009].

Using a Magnusson-Kligman GPMT procedure AKD as a 25% aqueous dispersion in paraffin oil showed a positive result. The test material was classified as a weak sensitiser. In a guinea pig maximisation test at an unspecified concentration AKD was classified to be non sensitising [ESIS 2009].

Two patch tests in human subjects with an unknown concentration of AKD were negative [ESIS, 2009].

### ***In Vitro* Toxicity Status**

#### **Carcinogenicity and mutagenicity**

When AKD was tested in the Ames assay with strains TA1535, TA100, TA1537 and TA98 to GLP no mutagenicity was detected at any of the concentrations tested (20, 200, 500, 2500 and 5000 µg/plate) either with or without metabolic activation [ESIS, 2009]

### **REFERENCES**

ESIS (2009) Searched on the European Chemicals Bureau website: IUCLID data sheet : 2-Oxetanone, 3-C12-16-alkyl 4-C13-17-alkylidene derivatives <http://ecb.jrc.it/ec.europa.eu/IUCLID-DataSheets/84989413.pdf>

Karademir A (2002). Quantitative determination of Alkyl ketene dimer retention in paper made on a pilot paper machine. Turk J Agric For 26: 253-260.