

A21M-005

## CAPROLACTONE MONOMER AS A SOLVENT

Caprolactone Monomer ( $\epsilon$ -Caprolactone) is the internal ester of hydroxy caproic acid and is a colourless, mobile liquid.

The lactone ring is relatively easily opened by compounds containing active hydrogen atoms, particularly alcohols. Elevated temperatures and catalysts are however normally required. Each ring opening step forms a terminal, primary hydroxyl group.

In addition to its interest as a chemical intermediate, Caprolactone Monomer is an excellent solvent.

### Typical Physical Properties

Boiling point	:	232°C
Melting point	:	-1°C
Viscosity, at 20°C	:	7 cp
Specific gravity, at 20°C	:	1.079
Flash point (closed cup)	:	235° - 240°F
Refractive index $n_{D20}$	:	1.4629

The product is supplied in 200 kilos nett steel or high density polyethylene drums, with the following typical analysis:-

Assay	:	99.9% min.
Acid value	:	0.2 mg KOH/g max.
Water content	:	0.015% max.

The product is hygroscopic and slowly hydrolyses in the presence of water. It should therefore be stored in sealed containers at all times.

## SOLVENT PROPERTIES

### 1. Miscibility with common solvents

Caprolactone is miscible with most liquid organic solvents and chemicals. The major exception is that of aliphatic hydrocarbons.

#### a) Aliphatic Hydrocarbons (and cycloaliphatics)

Caprolactone will form solutions with low levels of aliphatic hydrocarbons, e.g. 5% hydrocarbon. On heating it is possible to make a 50/50 solution with most aliphatics however on cooling separation occurs.

Solvents in this category include:

- 100-120 petroleum ether
- Cyclohexanone
- Methyl cyclohexanone
- Shellsol T
- Decalin

Insoluble hydrocarbons include liquid paraffin.

#### b) Aromatic Hydrocarbons

Caprolactone is completely miscible with most aromatic hydrocarbons.

These include:

- Benzene
- Toluene
- Xylene
- Ethyl Benzene
- Cumene
- Cymene
- Tetralin
- Methyl Naphthalene
- Aromasol H
- Styrene

#### c) Unsaturated Hydrocarbons (and Terpenes)

Caprolactone is miscible with the following:

- Cyclohexene
- Methyl Cyclohexene
- Dipentene
- Styrene

d) Nitro-compounds

Caprolactone is miscible with the following:

Nitromethane  
Nitropropane  
Nitrobenzene

e) Halogenated Hydrocarbons

Caprolactone is miscible with most members of this class:

Methylene Dichloride  
Chloroform  
Carbon tetrachloride  
Ethylene dichloride  
Trichloroethane  
Tetrachloroethane  
Trichloroethylene  
Perchloroethylene  
Chlorobenzene  
Dichlorobenzene  
Propylene Dichloride  
Benzyl Chloride  
Bromobenzene

f) Alcohols

Caprolactone is miscible with most members of this class, including most isomers of the following:

Methyl, Ethyl, Propyl, Butyl and Amyl Alcohols, also  
Benzyl Alcohol  
Cyclohexanol and Methyl cyclohexanol  
Diacetone Alcohol  
Allyl Alcohol  
2-ethyl hexanol  
n-decanol

g) Caprolactone is miscible with most ketones, including:

Acetone  
Methyl ethyl ketone  
Methyl isobutyl ketone  
Isophorone  
Cyclohexanone  
Methyl cyclohexanone  
Cyclopentanone  
Methyl iso-amyl ketone

h) Esters

Caprolactone is miscible with most of the esters, including:

Methyl acetate  
Ethyl acetate  
Amyl acetate  
Cyclohexyl acetate  
Methylcyclohexyl acetate  
di-n-butyl fumarate  
di-n-butyl maleate  
ethyl formate  
benzyl formate  
amyl formate  
di-ethyl adipate  
di-ethyl malonate  
di-n-butyl itaconate  
di-ethyl carbonate  
di-nonyl sebacate  
di-methyl phthalate  
di-butyl phthalate  
di-iso-octyl phthalate  
di-allyl phthalate  
methyl benzoate  
2-ethoxy ethyl acetate  
 $\gamma$ -butyrolactone  
Tri-ethyl phosphate

i) Glycols and glycol ethers

Caprolactone is completely miscible with most glycols and glycol ethers, including the following:

Ethylene glycol  
Digol and polyethylene glycols of all molecular weights (if liquid)  
Propylene glycol  
Polypropylene glycols of all molecular weights (if liquid)  
2-butoxy ethanol  
2-ethoxy ethanol  
2-methoxy ethanol  
2-ethoxy ethyl acetate

Exceptions include Glycerol (only soluble hot).

j) Ethers

Caprolactone is completely miscible with the following:

1,4 Dioxan  
Tetrahydrofuran  
Diethyl ether  
Di-isopropyl ether

### **Miscellaneous:**

Caprolactone is miscible with the following:

Carbon disulphide  
Dimethyl sulphoxide  
Water  
Pyridine  
Dimethyl Formamide  
Dimethyl acetamide  
N-methyl-2-pyrrolidone

### **2. Miscibility with common organic liquid chemicals not normally used as solvents**

Caprolactone is completely miscible with most liquids, including:

Acids such as formic, acetic, propionic, butyric, caproic, lactic, in fact all liquid organic acids.

Amines such as ethanolamine, diethanolamine, triethanolamine, ethylene diamine, diethylene triamine, triethylene tetramine, di-ethylamine, di-n-butylamine, cyclohexylamine, benzylamine.

Monomers such a vinyl acetate, acrylic acid, styrene, methyl methoxylate, ethyl acrylate, methyl acrylate, acrylamide, di-allyl phthalate, "penton" monomer (bis 3,3 chloromethyl oxetane).

Aldehydes such as acetaldehyde, benzaldehyde.

### **3. Solubility of common solid organic compounds in Caprolactone Monomer**

a) The following materials tested were insoluble, both hot and cold:

Starch  
Sucrose (chars on heating)  
Maltose (partially soluble hot)  
Mannitol (partially soluble hot)  
Glucose (partially soluble hot)

b) The following materials tested were soluble hot and cold:

p-phenylene diamine  
Benzoic acid  
Tartaric acid  
Citric acid  
Trimethylol Propane  
Long chain fatty acids <C12  
Dicyclohexyl phthalate  
Bisphenol A  
Maleic Anhydride  
Phthalic Anhydride  
Succinic Anhydride  
Toluene di-isocyanate  
MDI, e.g. PAPI, Suprasec DN, Isonate 143L  
IPDI adduct H3150  
Trimethylhexamethylene di-isocyanate

c) The following materials tested were soluble hot and insoluble cold:

Hexamine  
Fructose  
Pentaerythritol  
Long chain fatty acids >C12  
Cetyl alcohol  
Fumaric acid  
Isophthalic acid  
Adipic acid  
Paraformaldehyde

d) The following materials were insoluble hot and cold:

Melamine  
N-hydroxy methacrylamide

#### 4. Solubility of liquid resins in Caprolactone Monomer

Caprolactone dissolved all the liquid resins examined:

- a) Unsaturated polyesters: General purpose e.g. Crystic 65 PA  
Isophthalic type e.g. Crystic 491  
Bisphenol A type e.g. Crystic 600 PA  
Vinyl ester type e.g. Derakane 411/45  
Phenolic vinyl ester type,  
e.g. Derakane 470/36  
Hot press type e.g. Paraplex  
P-340
- b) Oil-free polyesters: Branched medium MW e.g. BA-500  
Solid linear medium MW e.g. LH-812  
Solid linear high MW e.g. L206
- c) Acrylic coating resins: Hydroxy acrylic e.g. H-230-XB  
Acrylamide acrylic e.g. A-160-XBN
- d) Formaldehyde types: Butylated UF e.g. BE 610  
Butylated MF e.g. BE 683  
Isobutylated PF e.g. PR 285  
HMMM e.g. BE 370
- e) Epoxies: e.g. Epikote 828
- f) Alkyds: e.g. Medium oil-length  
e.g. BA 549

#### 5. Solubility of solid resins in Caprolactone Monomer

The following categories were found:

Category		
1	Insoluble hot and cold.	
2	Insoluble cold - insoluble hot - precipitating on cooling.	
3	Insoluble cold - soluble hot - forms stable solution.	
4	Partially soluble hot and cold.	
5	Partially soluble cold - forms stable solutions on heating.	
6	Soluble hot and cold.	

Category    1    Insoluble hot and cold

Polyethylene  
 Polypropylene  
 Surlyn  
 Acetal Copolymer  
 Ethylene Vinyl Acetate (slightly soluble hot)  
 EPDM rubber stock  
 Polybutylene Terephthalate (slightly soluble hot?)  
 SBR rubber stock  
 Polyacrylamide  
 PTFE  
 Polyethylene Terephthalate (slightly soluble hot?)  
 Polyvinyl Alcohol (slightly soluble hot?)  
 Methyl Cellulose (may be partially soluble)

Category    2    Insoluble cold - soluble hot precipitating on cooling

Polyamides (dissolve above Mpt of polymer)  
 including Nylon 66, Nylon 6, Nylon 610, Nylon 11,  
 Nylon 12  
 Carnauba wax  
 Beeswax  
 Polybutadiene diols (RSM-4)  
 Poly (bis 33 chloromethyloxetane)  
 Hytrel 7246 and 4056 (polyester rubbers)

Category    3    Insoluble cold - soluble hot to form stable solution

Polymethyl methacrylate  
 Polycaprolactone (MW<sub>~</sub> 5,000 - 50,000)  
 Polyvinyl formal

Category    4    Partially soluble hot and cold - forms stable dispersion

ABS                    (T 100000)  
 PPO                    (Noryl)

Category    5    Partially soluble cold - forms stable solutions on heating

Polycarbonate (Lexan)  
 Polyarylate (Arylef U 100)  
 Ethyl Cellulose

Category    6    Completely soluble cold and hot

Cellulose acetate  
Cellulose acetate butyrate  
Polystyrene  
PVC            suspension grade  
PVC            emulsion grade  
PVC            copolymer  
PVC            plasticised compound  
Polyvinyl Butyral  
Polyvinyl Acetate  
Polyurethane rubber (thermoplastic Estane 58300)  
Nitrocellulose  
Polyethersulphone  
Polyvinyl Pyrrolidone  
Polypropylene Adipate  
Polypropylene glycol  
Polyethylene glycol  
Epoxy resins (Epikote 1004 and  
Epikote 1007)  
Perbunan N3302NS (Butyl rubber stock)  
Vamac N123 (ethylene acrylic rubber stock)

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