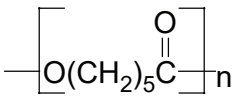
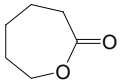
PCL poly(ε-caprolactone)

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	poly(ε-caprolactone)	
CAS name	-	2-oxepanone, homopolymer; poly[oxy(1-oxo-1,6-hexanediyl)]	
Acronym	-	PCL	
CAS number	-	24980-41-4; 25248-42-4	
Formula			
HISTORY			
Person to discover	-	Hostettler, F	Hostettler, F, US Patent 2,933,477, Union Carbide, Apr. 19, 1960.
Date	-	1960	
Details	-	polycaprolactone synthesis	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	502-44-3	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	114.14	
Method of synthesis	-	ring-opening addition polymerization of ε-caprolactone at 170°C under nitrogen with dibutyl stanneous oxide as the catalyst; also condensation of 6-hydroxycaproic acid gives PCL; polymerization is frequently conducted in extruder	Kim, B J; White, J L, Antec, 224-8, 2000; Labet, M; Thielemans, Chem. Soc. Rev., 38, 3484-3504, 2009.
Temperature of polymerization	°C	130	
Catalyst	-	99 (reactive extrusion)	Raquez, J-M; Degee, P; Dubois, P; Balakrishnan, S; Narayan, R, Polym. Eng. Sci., 45, 622-29, 2005.
Number average molecular weight, M_n	dalton, g/mol, amu	530-630,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	10,000-200,000	
Polydispersity, M_w/M_n	-	1.08-1.53	
STRUCTURE	-		
Crystallinity	%	57-76	Labet, M; Thielemans, Chem. Soc. Rev., 38, 3484-3504, 2009; Gumusderelioglu, M; Kaya, F B; Beskardes, I G, J. Colloid Interface Sci., 358, 444-53, 2011.
Cell type (lattice)	-	orthorhombic	
Cell dimensions	nm	a:b:c=0.745:0.498:1.705	
Number of chains per unit cell	-	4	
Chain conformation	-	nearly planar	
Rapid crystallization temperature	°C	58-150	
COMMERCIAL POLYMERS			
Some manufacturers	-	DOW; Solvay	

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PARAMETER	UNIT	VALUE	REFERENCES
Trade names	-	Tone; Capa	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.07-1.20	
Color	-	white	
Odor	-	odorless	
Melting temperature, DSC	°C	58-63	
Decomposition temperature	°C	200-220	
Glass transition temperature	°C	-60 to -72	
Heat of fusion	kJ mol^{-1}	8.9	
Contact angle of water, 20°C	degree	77-141 (advancing); 35-54 (receding)	Gumusderelioglu, M; Kaya, F B; Beskardes, I G, J. Colloid Interface Sci., 358, 444-53, 2011.
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	7.6-58	
Tensile modulus	MPa	200-1,380	
Elongation	%	300-600	
Flexural modulus	MPa	200-500	
Elastic modulus	MPa	237-288 (microfiber)	
Young's modulus	MPa	210-440	
Izod impact strength, notched, 23°C	J m^{-1}	120-375	Wei, X; Wong, S-C; Baji, A, Antec, 2737-41, 2009.
Viscosity number	ml g^{-1}	70-130	
Melt viscosity, shear rate=1000 s^{-1}	Pa s	1500	
CHEMICAL RESISTANCE			
Alcohols	-	good	
Aromatic hydrocarbons	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Good solvent	-	benzene, chloroform, dimethylacetamide, THF	
Non-solvent	-	methanol	
FLAMMABILITY			
Ignition temperature	°C	275	
Heat release	kJ g^{-1}	24.4	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Char at 500°C	%	0	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Heat of combustion	J g^{-1}	24,400	
BIODEGRADATION			
Typical biodegradants	-	*Pseudomonas, Alcanivorax*, and *Tenacibaculum*	Sekiguchi, T; Saika, A; Nomura, K; Watanabe, T; Watanabe, T; Fujimoto, Y; Enoki, M; Sata, T; Kato, C; Kanehiro, H, Polym. Deg. Stab., 96, 1397-1403, 2011.

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PARAMETER	UNIT	VALUE	REFERENCES
TOXICITY			
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
OSHA	mg m^{-3}	5 (respirable), 15 (total)	
Oral rat, LD_{50}	mg kg^{-1}	10,000	
PROCESSING			
Preprocess drying: temperature/ time/residual moisture	°C/h/%	compounding, extrusion, electrospinning, PU prepolymer synthesis	
Applications	-	fibers	
Outstanding properties	-	biodegradable	
BLENDS			
Suitable polymers	-	ABS, CB, NC, PC, PHB, PLA, PPy, PVC, starch	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C=O – 1778; C=C – 1642; C-O – 1164, 1107;	Vogel, C; Siesler, H W, Macromol. Symp., n265, 1483-94, 2008.