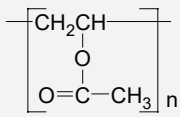
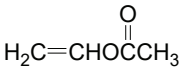
PVAc poly(vinyl acetate)

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	poly(vinyl acetate)	
IUPAC name	-	poly(ethenyl ethanoate)	
CAS name	-	acetic acid ethenyl ester, homopolymer	
Acronym	-	PVAc	
CAS number	-	9003-20-7	
EC number	-	203-545-4	
RTECS number	-	AK0920000	
Formula			
HISTORY			
Person to discover	-	Fritz Klatte	Klatte, F; Rollett, A, US Patent 1,241,738, 1917.
Date	-	1912	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	108-05-4	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	86.09	
Monomer ratio	-	100% or less (copolymers)	
Method of synthesis	-	oxidative addition of acetic acid to ethylene	
Catalyst	-	Pd; vanadium complex	Shaver, M P; Hanhan, M E; Jones, M R, Chem. Commun., 46, 2127-29, 2010.
Heat of polymerization	J g^{-1}	875-1,045	Joshi, R M, J. Polym. Sci., 56, 313, 1962.
Mass average molecular weight, M_w	dalton, g/mol, amu	13,000-500,000	
Polydispersity, M_w/M_n	-	2.0	
Polymerization degree (number of monomer units)	-	100-5000	
Molar volume at 298K	cm^3 mol^{-1}	calc.=74.25; 64.5 (crystalline); 72.4 (amorphous)	
Van der Waals volume	cm^3 mol^{-1}	calc.=45.9 (crystalline); 45.9 (amorphous)	
Radius of gyration	nm	66	Ahmed, I; Pritchard, J G; Blakely, C F, Polymer, 25, 4, 543-50, 1984.
End-to-end distance of unperturbed polymer chain	nm	170-380	Ahmed, I; Pritchard, J G; Blakely, C F, Polymer, 25, 4, 543-50, 1984.
STRUCTURE			
Crystallinity	%	amorphous	
Entanglement molecular weight	dalton, g/mol, amu	calc.=8667	

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COMMERCIAL POLYMERS			
Some manufacturers	-	Wacker	
Trade names	-	Vinnapearl	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.18-1.20	
Bulk density at 20°C	g cm^{-3}	0.7-0.85	
Color	-	colorless	
Refractive index, 20°C	-	1.467-1.469	
Odor		odorless	
Melting temperature, DSC	°C	152-180	
Softening point	°C	>190	
Decomposition temperature	°C	>250	
Fusion temperature	°C		
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	2.8E-4	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.159	
Glass transition temperature	°C	calc.=31; 28-32; 24-31 (atactic); 26 (isotactic); 28-40 (commercial)	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	20.9, 11.3, 9.7	
Interaction radius		13.7	
Hildebrand solubility parameter	$MPa^{0.5}$	calc.=19.2-20.93; exp.=18.0-25.7	
Surface tension	mN m^{-1}	36.5	
Dielectric constant at 100 Hz/1 MHz	-	-/3.5	
Dissipation factor at 1 MHz		150	
Permeability to oxygen, 25°C	cm^3 cm cm^{-2} s^{-1} Pa^{-1} x 10^{12}	0.0367	
Diffusion coefficient of oxygen	cm^2 s^{-1} $x10^6$	0.0562	
Contact angle of water, 20°C	degree	60.6	
Surface free energy	mJ m^{-2}	38.5	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	6.2-12	
Water absorption, equilibrium in water at 23°C	%	3-6	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	poor	
Alcohols	-	poor	
Alkalis	-	good	
Aliphatic hydrocarbons	-	fair	
Aromatic hydrocarbons	-	poor	

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PARAMETER	UNIT	VALUE	REFERENCES
Esters	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Θ solvent, Θ-temp.=29, 123, 19, 6°C	-	n-butyl ethyl ketone, cetyl alcohol, ethanol, methanol	
Good solvent	-	acetic acid, acetone, acetonitrile, allyl alcohol, chlorobenzene, chloroform, DMF, DMSO, metanol, THF, toluene	
Non-solvent	-	acids, diluted alkalis, carbon disulfide, cyclohexanol, ethylene glycol, mesitylene	
FLAMMABILITY			
Char at 500°C	%	1.2	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
WEATHER STABILITY			
Spectral sensitivity	nm	313	Ferreira, J L; Melo, M J; Ramos, A, Polym. Deg. Stab., 95, 453-61, 2010.
Products of degradation	-	chain scission, acetic acid	
BIODEGRADATION			
Typical biodegradants	-	plasticizers are attacked by fungi; hydrolysis by lipase	Domenech-Carbo, M T; Bitossi, G; de la Cruz-Canizares, J; Bolivar-Galiano, F; del Mar Lopez-Miras, M; Romero-Noguera, J; Martin-Sanchez, I, J. Anal. Appl. Pyrolysis, 85, 480-86, 2009; Chattopadhyay, S; Sivalingam, G; Madras, G, Polym. Deg. Stab., 80, 477-83, 2003.
TOXICITY			
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
Mutagenic effect	-	non-mutagenic	
Oral rat, LD_{50}	mg kg^{-1}	>25,000; 3,080 mg kg^{-1} day^{-1} (NOAEL)	
Skin rabbit, LD_{50}	mg kg^{-1}	non-irritant	
PROCESSING			
Typical processing methods	-	mixing/compounding	
Additives used in final products	-	Fillers: aluminosilicate, calcium carbonate, clay, mica, talc; Plasticizers: acetyl triethyl citrate, benzyl butyl phthalate, dibutyl phthalate, castor oil, dipropylene glycol dibenzoate, epoxidized soybean oil, ethylene and propylene glycols, glycerin, triethanolamine, triacetin, tributyl citrate, triethyl citrate; Antistatic: quaternary ammonium salt; Release: zinc stearate	
Applications	-	adhesives, paints, paper, production of poly(vinyl alcohol)	
BLENDS			
Suitable polymers	-	NR, PCL, PE, PEO, PHB, PLA, PMMA, PPy, PVC, PVF, PVOH, polyacrylate	

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ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C=O – 1737; C-H – 1375; O-C – 1020	Asensio, R C; San Andres Moya, M; de la Roja, J M; Gomez, M, Anal. Bioanal. Chem., 395, 2081-96, 2009.
Raman (wavenumber-assignment)	cm^{-1}/-	C-C – 1132; C=C – 1525	Blazevska-Gilev, J; Kupcik, J; Subrt, J; Vorlicek, V; Galikova, A; Pola, J, Polymer, 46, 8973-80, 2005.
NMR (chemical shifts)	ppm	H NMR: COOH – 8.76; OH – 5.61, 5.58	Chattopadhyay, S; Sivalingam, G; Madras, G, Polym. Deg. Stab., 80, 477-83, 2003.