PB 1,2-polybutylene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	1,2-polybutylene	
IUPAC name	-	poly(1-ethylethylene), poly(but-1-ene)	
CAS name	-	1-butene, homopolymer	
Acronym	-	PB	
CAS number	-	9003-28-5	
HISTORY			
Person to discover	-	Edwards, R W; Francis, A W; Eichenbaum, R; Ringelman, R E; Wu, W C L, 1968. Natta, G; Pino, P; Mazzanti, G, 1969. Klingensmith, G B; Higgins, T L, 1986.	Edwards, R W; Francis, A W; Eichenbaum, R; Ringelman, R E; Wu, W C L, US Patent 3,362,940, Mobil Oil Corp., Jan 9, 1968. Natta, G; Pino, P; Mazzanti, G, US Patent 3,435,017, Montecatini Edison, Mar. 25, 1969. Klingensmith, G B; Higgins, T L, US Statuatory Invention Registration H179, Dec. 2, 1986.
Date	-	1968; 1969; 1986	
Details	-	Edwards et al. patented stereoregular PB; Natta et al. patented isotactic PB; Klingensmith et al. patented elastomeric PB	
SYNTHESIS			
Monomer(s) structure	-	$H_2C=CHCH_2CH_3$	
Monomer(s) CAS number(s)	-	106-98-9	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	56.1	
Method of synthesis	-	addition polymerization; polymerization occurs on contact of monomer with Zigler-Natta catalyst	
Temperature of polymerization	°C	120	
Pressure of polymerization	MPa	7-15	
Catalyst	-	Ziegler-Natta, nickel-based	
Number average molecular weight, M_n	dalton, g/mol, amu	20,000-300,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	85,000-2,200,000	
Polydispersity, M_w/M_n	-	4-12	
Molar volume at 298K	$cm^3 mol^{-1}$	calc.=64.1; 59.5 (crystalline); 65.2 (amorphous); exp.=65.2	
Van der Waals volume	$cm^3 mol^{-1}$	calc.=40.9-41.1 (crystalline); 40.9 (amorphous)	
Radius of gyration	nm	13.7-16.3	
STRUCTURE			
Crystallinity	%	45-55 (conventional); 47-58 (form I); 38 (form II)	Klingensmith, G B; Higgins, T L, US Statuatory Invention Registration H179, Dec. 2, 1986; Abedi, S; Sharifi-Sanjani, N, J. Appl. Polym. Sci., 78, 2533-39, 2000; Maring, D; Meurer, B; Weill, J. Polym. Sci. B, 33, 1235-47, 1995.
Cell type (lattice)	-	hexagonal, tetragonal, orthorhombic	
Cell dimensions	nm	a:b:c=1.77:1.77:0.65 (hexagonal); 1.542:1.542:2.05 (tetragonal); 1.238:0.892:0.745 (orthorhombic)	

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PARAMETER	UNIT	VALUE	REFERENCES
Number of monomers per unit cell	-	18 (hexagonal); 44 (tetragonal)	Winkel, A K; Miles, M J, Polymer, 41, 2313-17, 2000.
Polymorphs	-	I (hexagonal; three-fold helix), I' (hexagonal); II (tetragonal; four-fold helix); III (orthorhombic; 2/1 helix)	Natta, G; Corradini, P; Bassi, I W, Rend. Accad. Naz. Lincei, 19, 404, 1955; Kim, K-W; Lee, K-H; Park, J-H; Lee, D-R; Ko, J-A; Kim, H-Y, Fibers Polym., 10, 5, 667-72, 2009.
Tacticity	%	84.5-99.5 isotactic	Klingensmith, G B; Higgins, T L, US Statuatory Invention Registration H179, Dec. 2, 1986.
Chain conformation	-	I (3/1 helix, twinned); I' (3/1 helix, untwinned); II (four 11/3 or 40/11 helix); III (2/1 helix)	Kim, K-W; Lee, K-H; Park, J-H; Lee, D-R; Ko, J-A; Kim, H-Y, Fibers Polym., 10, 5, 667-72, 2009.
Entanglement molecular weight	dalton, g/mol, amu	calc.=4,344	
Lamellae thickness	nm	27-31	Samon, J M; Schultz, J M; Hsiao, B S, Macromolecules, 34, 2008-11, 2001.
Heat of crystallization	kJ kg^{-1}	33.1-38.9	
Rapid crystallization temperature	°C	72	Maring, D; Meurer, B; Weill, J. Polym. Sci. B, 33, 1235-47, 1995.
Avrami constants, k/n	-	7.1E-2 to 1.98E-3/2.43-2.69	Maring, D; Meurer, B; Weill, J. Polym. Sci. B, 33, 1235-47, 1995.
COMMERCIAL POLYMERS			
Some manufacturers	-	LyondellBasell	
Trade names	-	PB	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	0.87-0.92; 0.95 (crystalline)	
Refractive index, 20°C	-	calc.=1.4669-1.5012; exp.=1.5125-1.5246	
Odor	-	odorless	
Melting temperature, DSC	°C	113-126; 97-142 (isotactic); 50 (syndiotactic); 120-135 (form I); 90-100 (form I'); 110-120 (form II); 90-100 (form III)	Shieh, Y-T; Lee, M-S; Chen, S-A, Polymer, 42, 4439-48, 2001.
Decomposition temperature	°C	300-440 (form I)	
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	1.1-6.7E-4	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.1344-0.22	
Glass transition temperature	°C	calc.=-23.0 to -60.0; exp.=-17.0 to -45.0; -20.5 (form I); -26.9 (form II)	Maring, D; Meurer, B; Weill, J. Polym. Sci. B, 33, 1235-47, 1995.
Specific heat capacity	J K^{-1} kg^{-1}	2,150-2,600	
Heat of fusion	kJ mol^{-1}	63-6.5	
Long term service temperature	°C	70 (lifetime of 50 years)	
Vicat temperature VST/A/50	°C	99	
Surface tension	mN m^{-1}	calc.=34.3-36.1	
Dielectric constant at 100 Hz/1 MHz	-	2.53	
Dissipation factor at 100 Hz	E-4	0.0005	
Dissipation factor at 1 MHz	E-4	0.0005	

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PARAMETER	UNIT	VALUE	REFERENCES
Permeability to oxygen, 25°C	cm^3 mm m^{-2} s^{-1} atm^{-1} day^{-1}	160	
Permeability to water vapor, 25°C	g m^{-2} 24h	29	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	27-45	
Tensile modulus	MPa	150-295	
Tensile stress at yield	MPa	12-15	
Elongation	%	200-400	
Flexural modulus	MPa	250-450	
Elastic modulus	MPa	290-295	
Poisson's ratio	-	calc.=0.393; exp.=0.47	
Shrinkage	%	2.5-5	
Brittleness temperature (ASTM D746)	°C	-18 to -20	
Intrinsic viscosity, 25°C	dl g^{-1}	0.0178-0.039	
Melt index, 190°C/10 kg	g/10 min	1-30	
Water absorption, 24h at 23°C	%	<0.03	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good	
Alcohols	-	good	
Alkalis	-	good	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Greases & oils	-	poor	
Halogenated hydrocarbons	-	good	
Ketones	-	poor	
Θ solvent, Θ-temp.=86	-	anisole	
Good solvent	-	benzene, chloroform, chlorobenzene, decalin, toluene	
Non-solvent	-	organic solvents	
FLAMMABILITY			
Ignition temperature	°C	>121	
Volatile products of combustion	-	CO, CO_2, toxic fumes	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	1/1/2	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
PROCESSING			
Typical processing methods	-	blown film, casting, extrusion, injection molding, rotational molding, spinning, thermoforming	

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PARAMETER	UNIT	VALUE	REFERENCES
Additives used in final products	-	Plasticizers: dioctyl adipate, phthalate, maleate, dibutyl phthalate, isodecyl pelargonate, oleyl nitrile, mineral oil, polybutene; Slip; Antiblock	
Applications	-	film, flexible piping, hot-melt adhesives, membranes, packaging, seals, shoe soles, wire & cable	
Outstanding properties	-	creep resistance, semi-crystalline	
BLENDS			
Suitable polymers	-	PE, PS, SBS	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	form I: 925 and 810; form I': 925 and 792; form II: 900; form III: 900 and 810	Abedi, S; Sharifi-Sanjani, N, J. Appl. Polym. Sci., 78, 2533-39, 2000.
x-ray diffraction peaks	degree	form I: 9.8, 17.1, 20; form III: 12.1, 17.0, 18.5	Kim, K-W; Lee, K-H; Park, J-H; Lee, D-R; Ko, J-A; Kim, H-Y, Fibers Polym., 10, 5, 667-72, 2009.