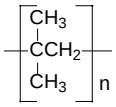
PIB polyisobutylene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polyisobutylene, polyisobutene	
IUPAC name	-	poly(2-methylpropene), polyisobutylene	
CAS name	-	1-propene, 2-methyl-, homopolymer	
Acronym	-	PIB	
CAS number	-	9003-27-4; 9003-29-6 (oligomers)	
RTECS number	-	UD1010000	
Linear formula			
HISTORY			
Person to discover	-	IG Farben	
Date	-	1931	
SYNTHESIS			
Monomer(s) structure	-	CH_2 H_3CCCH_3	
Monomer(s) CAS number(s)	-	115-11-7	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	56.11	
Monomer ratio	-	100%	
Number average molecular weight, M_n	dalton, g/mol, amu	180-6,000 (oligomers)	
Mass average molecular weight, M_w	dalton, g/mol, amu	900-1,100,000	
Polydispersity, M_w/M_n	-	1.06-2.10	
Molar volume at 298K	$cm^3 mol^{-1}$	calc.=59.2 (crystalline)	
Van der Waals volume	$cm^3 mol^{-1}$	calc.=40.9 (crystalline)	
Radius of gyration	nm	0.57 (M_w=390), 19.6 (4,040), 83.1 (73,200)	Frick, B; Dosseh, G; Cailliaux, A; Alba-Simionesco, C, Chem. Phys., 292, 311-23, 2003.
Chain-end groups	-	H, CH_2-CH=CH_2; Cl, COOH (derivatives)	Nagy, L; Palfi, V; Narmandakh, M; Kuki, A; Nyiri, A; Ivan, B; Zsuga, M; Keki, J. Am. Soc. Mass Spectrom., 20, 2342-51, 2009.
STRUCTURE			
Cell type (lattice)	-	orthorhombic	
Cell dimensions	nm	a:b:c=0.688:1.191:1.86	
Unit cell angles	degree	α:β:γ=90:90:90	
Number of chains per unit cell	-	4	
Chain conformation	-	helix	
Entanglement molecular weight	dalton, g/mol, amu	calc.=8,818	

PARAMETER	UNIT	VALUE	REFERENCES
COMMERCIAL POLYMERS			
Some manufacturers	-	BASF; INEOS	
Trade names	-	Oppanol; Indopol (oligomers)	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	0.788-0.921 (oligomers); 0.972 (crystalline)	
Color	-	clear to transparent	
Refractive index, 20°C	-	1.445-1.508 (oligomers); 1.5050-1.5100	
Odor	-	odorless	
Decomposition temperature	°C	>120	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.19-0.26	
Glass transition temperature	°C	calc.=-71; exp.=-72; -62 to -70	
Maximum service temperature	°C	-40 to 90	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	16.4, 1.7, 4.7; 16.9, 2.5, 4.0	
Interaction radius		7.9; 7.2	
Hildebrand solubility parameter	$MPa^{0.5}$	17.1	
Surface tension	mN m^{-1}	33.6	Roe, J R, J. Phys. Chem., 72, 2013, 1968.
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	42	
Contact angle of water, 20°C	degree	112.1	
Surface free energy	mJ m^{-2}	33.2	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	1.7-2.5	
Elongation	%	50-700	
Compression set, 24h 70°C	%	15	
Melt index, 230°C/3.8 kg	g/10 min	200-300	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good	
Alcohols	-	good	
Alkalis	-	good	
Aliphatic hydrocarbons	-	poor	
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Greases & oils	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Good solvent	-	benzene, carbon bisulfide, carbon tetrachloride, cyclohexanone, paraffin wax, toluene, xylene	
FLAMMABILITY			
Ignition temperature	°C	>40 to >280 (oligomers)	
Autoignition temperature	°C	>200	

PARAMETER	UNIT	VALUE	REFERENCES
Char at 500°C	%	0	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Volatile products of combustion	-	CO, CO_2, monomer and 52 more products	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004; Lehre, R S; Pattenden, Polym. Deg. Stab., 63, 321-40, 1999.
WEATHER STABILITY			
Important initiators and accelerators	-	ozone	
Products of degradation	-	hydroperoxides, radicals, ketones, carboxyl groups, hydroxyls, peresters, esters, lactones, chain scission, crosslinking, hydroxyls, double bonds	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0-1/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
Mutagenic effect	-	none	
Teratogenic effect	-	none	
Reproductive toxicity	-	none	
TLV, ACGIH	mg m^{-3}	2 (inhalable)	
Oral rat, LD_{50}	mg kg^{-1}	>2,000; >34,600	
Skin rabbit, LD_{50}	mg kg^{-1}	non-irritant	
ENVIRONMENTAL IMPACT			
Aquatic toxicity, Daphnia magna, LC_{50}, 48 h	mg l^{-1}	>1,000	
Aquatic toxicity, Fathead minnow, LC_{50}, 48 h	mg l^{-1}	>100	
Aquatic toxicity, Rainbow trout, LC_{50}, 48 h	mg l^{-1}	>1,000	
PROCESSING			
Typical processing methods	-	compounding, vulcanization, coating, sheeting	
Additives used in final products	-	Fillers: aluminum hydroxide, calcium carbonate, carbon black, cellulose, clay, kaolin, magnesium hydroxide, zinc oxide; Plasticizers: mineral oil, silicone oil, octyl palmitate	
Applications	-	cling film, glazing spacers, roofing membranes, sealants, transdermal administration of hypermic active substances	
BLENDS			
Suitable polymers	-	PE, PS	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	C-H – 1365, 1385; C=O – 1832, 1730, 1702	Small, C M; McNally, G M; Marks, A; Murphy, W R, Antec, 2882-86, 2002; Gonon, L; Troquet, M; Fanton, E; Gardette, J-L, Polym. Deg. Stab., 62, 541-49, 1998.