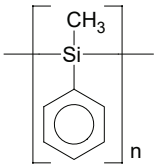
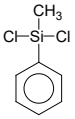
PMS poly(p-methylstyrene)

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	poly(p-methylstyrene)	
ACS name	-	benzene, 1-ethenyl-4-methyl homopolymer	
Acronym	-	PMS	
CAS number	-	24936-41-2	
Formula			
HISTORY			
Person to discover	-	Soday, F J	Soday, F J, US Patent 2,394,407, United Gas Improvement Company, Feb. 5, 1946.
Date	-	1946	
Details	-	polymerization of heat polymerizable aromatic olefins	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	622-97-9	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	118.2	
Monomer ratio	-	100%	
Method of synthesis	-	several methods can be used including: radical, anionic, and photoinitiated cationic polymerization	
Catalyst	-	titanium or zirconium compounds and methylalumoxane	
Heat of polymerization	J g^{-1}	283-330	Worsfold, D J; Bywater, S, J. Polym., Sci., 26, 299, 1957.
Number average molecular weight, M_n	dalton, g/mol, amu	28,000-141,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	25,000-293,000	
Polydispersity, M_w/M_n	-	1.0-4.3	
Molar volume at 298K	cm^3 mol^{-1}	calc.=113.2; 102.0 (crystalline); 111.0 (amorphous); exp.=115.0	
Van der Waals volume	cm^3 mol^{-1}	74.66; 78.0 (crystalline); 73.0 (amorphous)	
Molecular cross-sectional area, calculated	cm^2 x 10^{-16}	48.4	
STRUCTURE			
Crystallinity	%	20-30 (syndiotactic)	
Cell type (lattice)	-	orthorhombic	
Cell dimensions	nm	a:b:c=1.336:2.321:0.512 (form III)	De Rosa, C; Petraccone, V; Guerra, G, Polymer, 37, 23, 5247-53, 1996.

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PARAMETER	UNIT	VALUE	REFERENCES
Unit cell angles	degree	α:β:γ=90:90:90	
Number of chains per unit cell	-	6	
Crystallite size	nm	3 (length of form III)	de Ballesteros, O R; Auriemma, F; De Rosa, C; Floridi, C; Petraccone, V, Polymer, 39, 15, 3523+28, 1998.
Polymorphs	-	I, II, III, IV, V	Rizzo, P; de Ballesteros, O R; De Rosa, C; Auriemma, F; La Camera, D; Petraccone, V; Lotz, B, Polymer, 41, 3745, 49, 2000.
Tacticity	%	95 (syndiotactic)	Esposito, G; Tarallo, O; Petraccone, V; Eur. Polym. J., 43, 1278-87, 2007.
Chain conformation	-	helical s(2/1)2 (I, II) (minimum energy conformation); transplannar (III, IV,V)	Esposito, G; Tarallo, O; Petraccone, V; Eur. Polym. J., 43, 1278-87, 2007.
Space group		Pnam (form III)	de Ballesteros, O R; Auriemma, F; De Rosa, C; Floridi, C; Petraccone, V, Polymer, 39, 15, 3523+28, 1998.
Entanglement molecular weight	dalton, g/mol, amu	calc.=13,477	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	1.01-1.04	
Color	-	white	
Refractive index, 20°C	-	calc.=1.5921-1.595; exp.=1.5874-1.610	
Odor	-	odorless	
Melting temperature, DSC	°C	225	
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	6.6-7.1E-4	
Thermal conductivity, melt	W m^{-1} K^{-1}	0.1323	
Glass transition temperature	°C	calc.=81-126; exp.=93-110; 113 (atactic)	Camelio, P; Lazzeri, V; Waegell, B; Cypcar, C; Mathias, L J, Macromolecules, 31, 2305-11, 1998.
Heat deflection temperature at 1.8 MPa	°C	92	
Hildebrand solubility parameter	$MPa^{0.5}$	calc.=19.33	
Surface tension	mN m^{-1}	calc.=38.8-48.6, exp.=38.7	
Surface free energy	mJ m^{-2}	38.7	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Poisson's ratio	-	0.341-0.345	
Melt index, 230°C/3.8 kg	g/10 min	5	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good	
Alcohols	-	very good	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	good	

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PARAMETER	UNIT	VALUE	REFERENCES
Θ solvent, Θ-temp.=34.3, 10, 85°C	-	cyclohexane, *trans*-decalin, n-hexyl acetate	
Good solvent	-	benzene, butyl acetate, carbon disulfide, chlorinated aliphatic hydrocarbons, chloroform, cyclohexanone, dioxane, ethyl acetate, ethylbenzene, MEK, NMP, THF	
Non-solvent	-	acetic acid, acetone, alcohols, ethyl ether, saturated hydrocarbons	
FLAMMABILITY			
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, and more in ref.	Zuev, V V; Bertini, F; Audisio, G, Polym. Deg. Stab., 71, 213-21, 2001.
WEATHER STABILITY			
Activation wavelengths	nm	265	
Excitation wavelengths	nm	294, 336, 425	Al Ani, K E; Ramadhan, A E, Polym. Deg. Stab., 93, 1590-96, 2008.
Products of degradation	-	chain scission	
TOXICITY			
HMIS: Health, Flammability, Reactivity rating	-	0/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
BLENDS			
Suitable polymers	-	PC, PMMA, PS	
ANALYSIS			
NMR (chemical shifts)	ppm	C NMR: quaternary carbon – 142.3; phenyl carbons – 126.8, 127.7, 133.8; CH – 39.9; CH_2 – 43.2; CH_3 – 20.2	Zhang, X; Yan, W; Li, H; Shen, X, Polymer, 46, 11958-61, 2005.