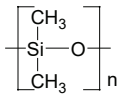
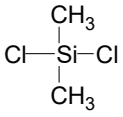
PDMS polydimethylsiloxane

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polydimethylsiloxane	
CAS name	-	poly[oxy(dimethylsilylene)]; poly[oxy(dimethylsilylene)], α-(trimethylsilyl)-omega-[(trimethylsilyl)oxy]-	
Acronym	-	PDMS	
CAS number	-	9016-00-6; 42557-10-8	
EC number	-	226-171-3	
RTECS number	-	TQ2690000	
Formula			
HISTORY			
Person to discover	-	Frederick Stanley Kipping	
Date	-	1901-1930; 1935	
Details	-	Kipping developed foundations of organosilicone chemistry and technology; first practical application of silicones in 1935	
SYNTHESIS			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	1066-35-9	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	94.62	
Monomer ratio	-	100%	
Method of synthesis	-	the direct reaction between silicon metal and methyl chloride in a fluid bed reactor yields a complex mixture of methyl chlorosilanes; the chlorosilanes are distilled or purified, and the primary product - dimethyldichlorosilane, $(CH_3)_2SiCl_2$ – is reacted with water (hydrolysis) to give poly(dimethylsiloxane) oligomers: $[Me_2SiO]_n$.	
Catalyst	-	DOTM	
Cure mechanism		acetoxy, neutral, neutral catalytic (moisture cured systems)	
Number average molecular weight, M_n	dalton, g/mol, amu	300-66,000	
Mass average molecular weight, M_w	dalton, g/mol, amu	500-423,000	
Polydispersity, M_w/M_n	-	1.6-3.9	
Molar volume at 298K	cm^3 mol^{-1}	69.1 (crystalline)	
Van der Waals volume	cm^3 mol^{-1}	47.6 (crystalline)	
Radius of gyration	nm	1-1.2; 3.1 (partially crosslinked); 5.5-6.1 (final crosslink density in membrane)	Jadav, G L; Aswal, V K; Singh, P S, J. Membrane Sci., in press, 2011; Serbescu, A; Saalwaechter, K, Polymer, 50, 5434-42, 2009.

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Chain-end groups	-	methyl, vinyl, hydrogen, hydroxyl	Mrozek, R A; Cole, P J; Otim, K J; Shull, K R; Lenhart, J L, Polymer, in press, 2011; Jadav, G L; Aswal, V K; Singh, P S, J. Membrane Sci., in press, 2011.
STRUCTURE			
Crystallinity	%	24-95 (depends on cooling rate); 0-14 (with 10-40% fumed silica)	Aranguren, M I, Polymer, 39, 20, 4897-4906, 1998.
Cell type (lattice)	-	monoclinic	
Cell dimensions	nm	a:b:c=1.3:0.775:0.83	
Unit cell angles	degree	α:β:γ=90:60:90	
Entanglement molecular weight	dalton, g/mol, amu	calc.=8,160; exp.=21,000-33,000	
Rapid crystallization temperature	°C	-56 to -65	
COMMERCIAL POLYMERS			
Some manufacturers	-	Dow Corning	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	0.97; 0.98 (amorphous); 1.07 (crystalline)	
Color	-	clear fluid	
Refractive index, 20°C	-	1.375-1.404; 1.4-1.5 (LED applications)	
Gloss, 60°, Gardner (ASTM D523)	%	47	
Odor	-	odorless	
Melting temperature, DSC	°C	-35 to -55	
Decomposition temperature	°C	>343 (silicone oil); 235 (sealant)	
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	9.0-9.6E-4	
Thermal conductivity, 15-80°C	W m^{-1} K^{-1}	0.151-0.167; 0.15-1 (sealants); 1.9-6.8 (specially formulated thermally conductive adhesives and greases)	
Glass transition temperature	°C	-123 to -127; -121 to -122 (with 10-40% fumed silica)	Aranguren, M I, Polymer, 39, 20, 4897-4906, 1998.
Specific heat capacity	J K^{-1} kg^{-1}	1,350-1,700	
Maximum service temperature	°C	350 (coatings, up to 1000 h); -40 to 260 (lead-free solder reflow)	
Long term service temperature	°C	-45 to 150 (sealants); -55 to 200 (coatings)	
Hildebrand solubility parameter	$MPa^{0.5}$	14.9-15.6	
Surface tension	mN m^{-1}	20.3-21.5	
Dielectric constant at 100 Hz/1 MHz	-	2.8	
Dissipation factor at 100 Hz	-	0.00012-0.001	
Volume resistivity	ohm-m	4E13	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	12-27	
Contact angle of water, 20°C	degree	107-110	
Surface free energy	mJ m^{-2}	20.4	
Speed of sound	m s^{-1}	837-987	

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PARAMETER	UNIT	VALUE	REFERENCES
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	0.5-9.7	
Tensile modulus	MPa	0.69-3.45	
Elongation	%	220-1,600	
Tear strength	kN m^{-1}	5-40	
Tension adhesion	MPa	1.2	
Peel strength	kg cm^{-1}	2.7-7.1	
Poisson's ratio	-	0.5	
Shore A hardness	-	15-70	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	good	
Alcohols	-	fair-poor	
Alkalis	-	good	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good-poor	
Greases & oils	-	good	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Other	-	poor	
Θ solvent, Θ-temp.=-5.2, -38.2, -81.4, 4.8°C	-	benzene, n-butyl acetate, cyclohexane, ethyl acetate	
Good solvent	-	amyl acetate, chlorobenzene, chloroform, cyclohexyl acetate, dichlorobenzene, ethyl bromide, ethyl acetate, hydrocarbons, trichloroethylene	
Non-solvent	-	acetone, acetonitrile, acetophenone, benzyl alcohol, benzyl acetate, gamma-butyrolactone, cyclohexanone, cyclohexanol, dichlorobenzene, dioxane, diphenyl oxide, ethyl formate, ethyl benzoate, methanol, nitrobenzene	
FLAMMABILITY			
Ignition temperature	°C	>320 (silicone oil), >100 (sealant)	
Autoignition temperature	°C	418-490	
Limiting oxygen index	% O_2	26-42	
Heat of combustion	J g^{-1}	19,530	Walters, R N; Hacket, S M; Lyon, R E, Fire Mater., 24, 5, 245-52, 2000.
Volatile products of combustion	-	CO, CO_2, SiO_2	
WEATHER STABILITY			
Spectral sensitivity	nm	300-350	
Activation wavelengths	nm	318, 325, 330, 360	
Transmittance	%	100 – 76.5; 300 nm – 44.8	Matsuzawa, N N; Oizumi, H; Mori, S; Irie, S; Shirayone, S; Yano, E; Okazaki, S; Ishitani, S; Dixon, D A, Jpn. J. Appl. Phys., 38, 7109-13, 1999.
Important initiators and accelerators	-	benzophenone, nitronous oxide, flame retardants containing halogens, ozone, stress	

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Products of degradation	-	hydrogen, water, carbon dioxide, ketone, unsaturations, hydroperoxides, radicals, chain scissions, crosslinks, quinomethane structures, benzene, acetophenone, benzaldehyde, benzene, formic acid, acetic acid, benzoic acid, conjugated double bonds	
Stabilizers	-	UVA: 2,4-dihydroxybenzophenone; 2-(2H-benzotriazol-2-yl)-p-cresol; 2-(2H-benzotriazole-2-yl)-4,6-di-tert-pentylphenol; 2-(2H-benzotriazole-2-yl)-4-(1,1,3,3-tetraethylbutyl)phenol; HAS: 1,3,5-triazine-2,4,6-triamine, N,N'''[1,2-ethanediyl-bis[[[4,6-bis[butyl(1,2,6,6-pentamethyl-4-piperidinyl) amino]-1,3,5-triazine-2-yl]imino]-3,1-propanediyl]bis[N',N''-dibutyl-N',N''-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-; bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate; 2,2,6,6-tetramethyl-4-piperidinyl stearate	
BIODEGRADATION			
Colonized products		coatings, dental materials, insulating rubber, medical devices, mortar protective coatings, sealants, stone protective coating	
Typical biodegradants	-	fungal growth decreases hydrophobicity of silicone products	
Stabilizers	-	2,3,5,6-tetrachloro-4-methylsulfonyl-pyridine, 2,3,5,6-tetrachloro-4-methylsulfonylpyridine, N-chloramine, sodium benzoate, triclosan, zosteric acid	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	1/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
Reproductive toxicity	-	adverse reproductive effects have occurred in experimental animals	
Oral rat, LD_{50}	mg kg^{-1}	>4990	
Skin rabbit, LD_{50}	mg kg^{-1}	>18,400	
ENVIRONMENTAL IMPACT			
Aquatic toxicity, *Rainbow trout*, LC_{50}, 48 h	mg l^{-1}	>10,000	
Mean degradation half-life	months	1-2 (coatings)	
PROCESSING			
Typical processing methods	-	calendering, casting, compression molding, extrusion, injection molding, room temperature, moisture or chemical cure of premixed compounds, transfer molding, vulcanization	
Processing temperature	°C	200-316 (vulcanization); 0-50 (moisture cure); 250-500 (extrusion vulcanization); 180-200 (continuous vulcanization in steam); 60-90 followed by 130-200 (peroxide cure)	
Processing pressure	MPa	3.45-13.78 (injection)	
Process time	s	5-10 (injection time); 30-90 (molding time for peroxide cured)	

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Additives used in final products	-	Fillers: aluminum oxide, aluminum powder, boron nitride, calcium carbonate, carbon black, carbon nanotubes, fumed silica, glass beads, metal powders, mica, montmorillonite, nano-$CaCO_3$, nanosilica, precipitated silica, silver, spherical alumina, zinc oxide; Plasticizers: acetyl triethyl citrate, diethylene glycol dibenzoate, dimethylsiloxane oligomer, epoxidized soybean oil, ethylene or propylene glycols, glycerin, hydroxy-terminated polydimethylsiloxane, phthalates, polyisobutylene, silicone oil, tricresyl phosphate, tripropylene glycol monoethyl ether; Antistatics: acicular conductive titanium oxide, acrylamidoamidosiloxane, chitin, graphite, nickel, silver, sulfonated silicone; Antiblocking: ailica; Release: PDMS compounds; Slip: silicone fluid; Peroxides (benzoyl peroxide or 2,4-dichlorobenzoyl peroxide); Thickener (polyacrylic acid polymers, e.g., Carbopol, hydroxyethyl cellulose); Surfactant (e.g., cocoamidopropyl betaine, amine type, sorbitan monoisostearate); Silicone oil (improves gloss, scratch resistance, etc.); Solvent (e.g., heptane, Exxsol); Wax, (e.g., carnauba, paraffin)	
Applications	-	automotive (shaft sealing rings, spark plug caps, o-rings, gaskets, ignition cables, coolant and heater hose), caulking and sealants, coatings, cookware, conductive rubber, defoaming, door and windows seal, drycleaning, electronics, firestops, general tubing, heat dissipative grease, lubricants, medicine, moldmaking, personal care, toys, transfusion and dialysis tubing, waveguide	
BLENDS			
Suitable polymers	-	PC, PET, TPU	
ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	ester linkage – 1720; CH=CH – 1600; Si-C – 1374	Rao, H; Zhang, Z; Song, C; Qiao, T, Reactive Functional Polym., 71, 537-43, 2011.
Raman (wavenumber-assignment)	cm^{-1}/-	Si-O-Si – 437-441; C-H – 1567	Lin, L-H; Liu, H-H; Hwang, J-J; Chen, K-M; Chao, J-C, Mater. Chem. Phys., 127, 248-52, 2011.