

Table S2. Analysis of existing test data for physicochemical properties

Item	Required data available as existing test data (%)				
	Total	Reliability 1	Reliability 2	Reliability 3	No data
State of substance	510 (100)	3 (0.5)	391 (76.7)	0 (0.0)	116 (22.7)
Melting point/freezing point	510 (100)	15 (2.9)	368 (72.2)	2 (0.4)	125 (24.5)
Boiling point	510 (100)	7 (1.4)	314 (61.6)	2 (0.4)	187 (36.7)
Relative density	510 (100)	6 (1.2)	212 (41.6)	6 (1.2)	286 (56.1)
Vapor pressure	510 (100)	15 (2.9)	317 (62.2)	1 (0.2)	177 (34.7)
Solubility	510 (100)	19 (3.7)	377 (73.9)	1 (0.2)	113 (22.2)
Grain size analysis	510 (100)	1 (0.2)	0 (0.0)	0 (0.0)	509 (99.8)
Octanol-water partition coefficient	510 (100)	31 (6.1)	257 (50.4)	0 (0.0)	222 (43.5)
Dissociation constant	510 (100)	2 (0.4)	104 (20.4)	0 (0.0)	404 (79.2)
Viscosity	510 (100)	0 (0.0)	158 (31.0)	0 (0.0)	352 (69.0)
Inflammability	510 (100)	16 (3.1)	238 (46.7)	13 (2.5)	243 (47.6)
Explosiveness	510 (100)	5 (1.0)	318 (62.4)	8 (1.6)	179 (35.1)
Oxidative degree	510 (100)	3 (0.6)	289 (56.7)	7 (1.4)	211 (41.4)
Total	6630 (100)	123 (1.9)	3343 (50.4)	40 (0.6)	3124 (47.1)