Isocyanato-terminated mono-urea of TDI

Amino-terminated mono-urea of TDI

Isocyanato-terminated mono-urea of 4,4’-MDI

Amino-terminated mono-urea of 4,4’-MDI

Property	Method	Notes	NCO-terminated mono-urea of TDI	NH_2-terminated mono-urea of TDI	NCO-terminated mono-urea of 4,4'-MDI	NH_2-terminated mono-urea of 4,4'-MDI
CASRN						
Physicochemical properties						
Vapor pressure at 25 °C [Pa]	Estimation EPI Suite MPBWIN v1.43		7.0×10^{-7}	1.1×10^{-7}	2.6×10^{-11}	5.0×10^{-12}
Melting point [°C]	OECD 102 (DTA/DSC)		193	196	203	200
Water solubility at 20 °C [mg/L]	OECD 105		0.020	56	<0.002	39 (pH 2) <0.004 (pH≥7)
Acid dissociation constant (pK_a) terminal amino group	Estimation EPI Suite KOWWIN v1.68	Cannot be measured – insoluble in water	Not applicable	4.6 +/- 0.1	Not applicable	5.1 +/- 0.3
Acid dissociation constant (pK_a) urea group	Estimation EPI Suite KOWWIN v1.68	Cannot be measured – insoluble in water	0.7 (NH_2^+ →NH) 13.7 (NH → N^-)	Not determined	Not determined	14.2 (NH → N-)
Octanol-water partition coefficient (log Pow) at 25 °C	OECD 117 (TDI) EPI Suite KOWWIN v1.68 (MDI)	Measurement unsuccessful for MDI-urea	3.7-4.7 (depending on isomer)	1.3-1.4 (depending on isomer)	8.2	3.3

Property	Method	Notes	NCO-terminated mono-urea of TDI	NH_2-terminated mono-urea of TDI	NCO-terminated mono-urea of 4,4'-MDI	NH_2-terminated mono-urea of 4,4'-MDI
Acute toxicity information						
Ready Biodegradability	OECD 301F	Not readily biodegradable				
72 h Algae Growth Inhibition [mg/L]	OECD 201	ErL_{50} EC_{50} NOELR NOEC	>100 >100 	 >100 >100	>100 >100 	 >100 >100
48 h Daphnia magna Immobilization [mg/L]	OECD 202	EL_{50} EC_{50}	>100 	 >100	>100 	 >100
96 h Danio rerio Lethality [mg/L]	OECD 203	LL_{50} EC_{50}	>100 	 >100	>100 	 >100
Acute oral toxicity in rat [mg/kg_{bw}]		(Steinhoff, 1973)	Not determined	>15000	Not determined	>15000

Summarized from 11700, 11729, 11741, 10658.