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3a,4,5,6,7,8,9,10,11,12,13,13a-Dodecahydro-3-(4-chlorophenyl)cyclododeca[d]isoxazole

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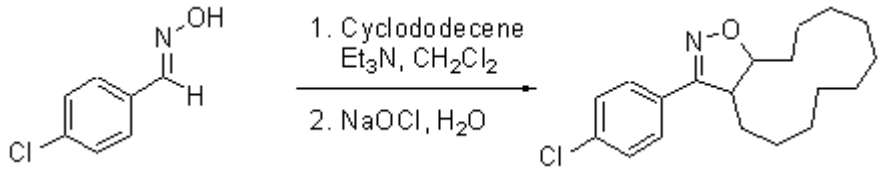

To a solution of 4-chlorobenzaldehyde oxime (0.40g) in CH_2Cl_2 (10 mL) in a large test-tube were added 1.0 mL of cyclododecene and 3 drops of triethylamine. The solution was cooled to 5°C, then 7.0 mL of 5% NaOCl solution in water was added in small portions. After each portion was added, the test-tube was agitated with a Vibromixer™ stirrer for 15 seconds. After the addition of all of the NaOCl solution, the test-tube was agitated with a Vibromixer™ stirrer for 15 seconds every 5 minutes over the next hour. The reaction mixture was allowed to stand at least overnight. The layers were separated, and the aqueous layer was extracted with CH_2Cl_2 (5 mL). The combined CH_2Cl_2 layers were evaporated to yield an off-white solid. The solid was recrystallized from 95% ethanol to yield shiny white flakes. Yield: 0.24g (29%).

M.p. 118-119°C.

IR (KBr pellet, cm^{-1}): 2936, 2855, 1590, 1494, 1469, 1446, 1404, 1346, 1093, 901, 868, 832.

^{1}H-NMR (300MHz, $CDCl_3$, ppm): 1.35-1.65 (20 H, multiplets), 3.48 (1H, d of m), 4.76 (1H, d of m), 7.38 (2H, m), 7.64 (2H, m).

^{13}C-NMR (75.5 MHz, $CDCl_3$, ppm): 159.0, 136.0, 129.4, 128.5, 128.2, 84.5, 48.4, 31.9, 29.9, 27.3, 27.1, 24.0, 23.4, 23.0, 22.4, 22.06, 22.00.

GC-MS (ion trap, m/e, in order of decreasing peak size): 137 (100%), 102, 50, 75, 139, 51, very small molecular ion at 319/321 detected.

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Sample Availability: available from MDPI.