1-ethoxycarbonylmethyl-3-(ethoxycarbonylmethylene)-2-oxo quinoxaline

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The compound 3, which exists in tautomeric equilibria between enamine (form A) and methylene imine (form B), was prepared by addition of ethoxycarbonylmethyl chloride 2 (1.23g, 0.01 mol) to a solution of 3-(ethoxycarbonylmethylene)-2-oxo quinoxaline, 1 [1] (2.32 g, 0.01 mol) in 60 ml DMF, K$_2$CO$_3$ (1.38g, 0.01mol) and triethylbenzylammonium chloride (0.001 mol). The mixture was stirred for 24 hours at room temperature. After filtration, the solvent was evaporated and the residue was recrystallized from ethanol affording 3 in 90% yield.

Melting point: 154-156°C.

IR (KBr, cm$^{-1}$): 1650 (\(\nu_{N-C=O}\)); 1720 (\(\nu_{N-C=O}\)).

$^1$H-NMR (250 MHz, CDCl$_3$): $\delta$= 11.20 (0.5H, s, NH, form A); 7.87-6.82 (8H, m, ar); 5.83 (0.5H, s, =CH, form A); 5.01 (1H, s, NCH$_2$); 4.89 (1H, s, NCH$_2$); 4.21 (8H, m, CH$_2$); 3.95 (2H, s, CH$_2$, form B); 1.27 (12H, m, CH$_3$).

$^{13}$C-NMR (250MHz, CDCl$_3$): $\delta$= 170.7 (Cq); 169.3 (Cq); 167.3 (Cq); 166.9 (Cq); 156.4 (Cq); 154.4 (Cq); 142.5 (Cq); 132.7 (Cq); 130.6 (CH$_{ar}$); 130.4 (CH$_{ar}$); 126.0 (Cq); 124.5 (CH$_{ar}$); 124.0 (CH$_{ar}$); 122.5 (CH$_{ar}$); 115.4 (CH$_{ar}$); 113.8 (CH$_{ar}$); 113.2 (CH$_{ar}$); 86.7 (=CH form A); 62.1 (CH$_2$); 62.0 (CH$_2$); 62.2
(CH₂); 59.9 (CH₂); 44.0 (NCH₂); 43.6 (NCH₂); 40.7 (CH₂ form B); 14.4 (CH₃); 14.1 (CH₃).

MS (LE): 318 [M⁺].

Reference

Sample Availability: Available from MDPI.

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