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N-(2,6-Dimethylphenyl)-2-(2-oxo-1-pyrrolidin-1-yl)-acetamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.121
Data-to-parameter ratio = 9.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{14}H_{18}N_2O_2$, a derivative of pyrrolidone, was synthesized by *N*-acylation and *N*-alkylation reactions, with 2,6-xylidine as the starting material. In the crystal structure, there is an intermolecular N—H···O hydrogen bond.

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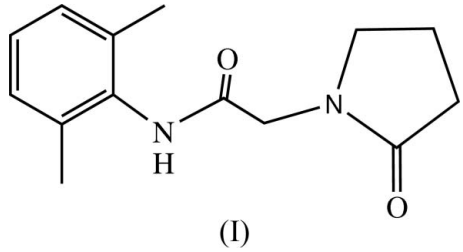
Comment

2-Pyrrolidones represent an important class of five-membered heterocycles. Pyrrolidone derivatives are of great interest because of their biological properties. Some derivatives of pyrrolidone improve cerebral functions (Kamihara *et al.*, 1995). Some show high efficacy as antidementia agents (Kisofukushima *et al.*, 1990). The title compound, (I), is one of the efficient drugs for the treatment of Alzheimers disease (Rene *et al.*, 2001). The molecular structure of (I) is shown in Fig. 1. In the crystal structure, there is an intermolecular N—H···O hydrogen bond (Table 1).



(I)

Experimental

2,6-Xylidine (20 mmol) was dissolved in toluene (300 ml), and sodium carbonate (15 mmol) was dissolved in water (100 ml). The two solutions were combined and chloroacetyl chloride (15 mmol) was added in a nitrogen stream at room temperature, followed by stirring for 2 h. 2-Pyrrolidone (30 mmol) and sodium amide (8 mmol) were then added slowly dropwise. After stirring the mixture at 333–343 K for 5 h, hot water (50 ml) was added and the mixture was allowed to cool with stirring. The crystals precipitated in the aqueous layer were recovered by filtration and dried under reduced pressure to obtain the title compound. The pure compound was obtained by recrystalization from ethyl acetate. Crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{14}H_{18}N_2O_2$
M_r = 246.30
Orthorhombic, $P2_12_12_1$
a = 6.3390 (13) Å
b = 9.3130 (19) Å
c = 22.712 (5) Å
V = 1340.8 (5) Å^3
Z = 4
D_x = 1.220 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, white
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.966, T_{max} = 0.989
3018 measured reflections
1545 independent reflections
1114 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.121
S = 1.02
1545 reflections
170 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.07P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.025 (4)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.80 (3)	2.07 (3)	2.846 (3)	165 (3)

Symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

H atoms bonded to C atoms were positioned geometrically at distances of 0.93–0.96 Å and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate but not to tip. The amide H atom was refined freely. In the absence of anomalous scatterers, Friedel pairs were merged.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

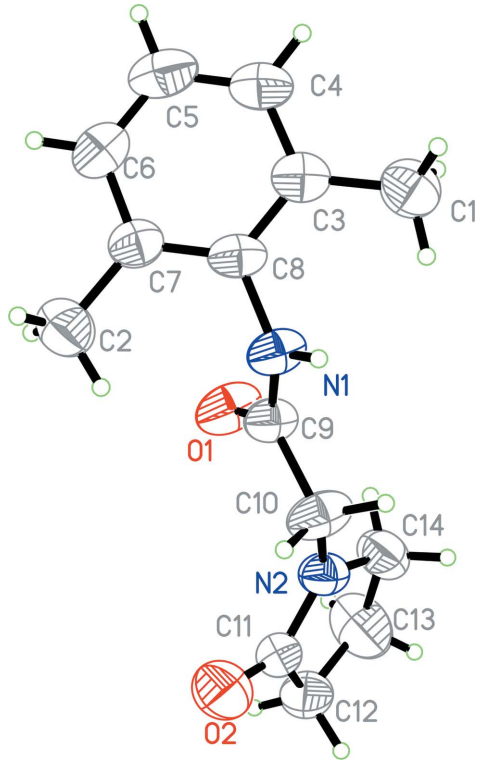


Figure 1
A view of the molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability.

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