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(*R*)-3-[(*E*)-3-(2-Furyl)acryloyl]-5,5-dimethyl-4-phenyloxazolidin-2-one

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Key indicators

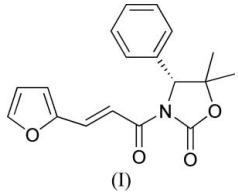
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.085
Data-to-parameter ratio = 9.4

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

The title compound, $C_{18}H_{17}NO_4$, posesses normal geometrical parameters. It was prepared as a key intermediate in the synthesis of enantiomerically pure 2-amino-3-(2-furyl)pentanoic acid *via* a Knoevenagel E reaction.

Comment

Aromatic ring-substituted amino acids can provide valuable tools in developing highly selective peptide ligands with specific structural features. In addition, they can provide a large lipophilic surface for binding to receptors, and for crossing membranes (Wang *et al.*, 2001). As part of our own work in this area, we prepared the title compound, (I), as an intermediate in the synthesis of the amino acid 2-amino-3-(2-furyl)pentanoic acid using the so-called Davies 'SuperQuats' chiral auxiliary (4*R*)-5,5-dimethyl-4-phenyloxazolidin-2-one (Davies & Sanganee, 1995; Bull *et al.*, 2000).



(I)

In the structure of (I) (Fig. 1), atom C3 is the chiral centre. The *R* configuration was assigned based on that of the equivalent atom in the starting material All the bond lengths and angles in (I) are within their expected ranges. The dihedral angle between the mean planes of the C3/N1/C1/O4/C2 ring and the C6–C11 benzene ring is 72.02 (5)°. The crystal packing of (I) is stabilized only by van der Waals forces.

Experimental

(*E*)-3-(2-Furyl)acrylic acid (5 g, 36 mmol) was coupled with optically pure (4*R*)-5,5-dimethyl-4-phenyloxazolidin-2-one (5.75 g, 30 mmol), and purification by column chromatography yielded an off-white solid in 81% yield. Crystals of (I) were recrystallized from a 1:8 EtOAc/hexane mixture (m.p. 411 K). ESI–MS calculated for $C_{18}H_{17}NO_4$: 311 (M^+); found: 334 (M^+ + Na).

Crystal data

$C_{18}H_{17}NO_4$
M_r = 311.33
Monoclinic, $P2_1$
a = 5.5281 (4) Å
b = 12.8677 (9) Å
c = 11.0920 (9) Å
β = 92.953 (3)°
V = 787.97 (10) Å^3
Z = 2
D_x = 1.312 Mg m^{-3}
Mo *Kα* radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
Block, colorless
0.30 × 0.27 × 0.24 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.924, T_{max} = 0.949
6973 measured reflections
1958 independent reflections
1859 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 28.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.04
1958 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.0655P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.041 (6)

In the absence of significant anomalous dispersion effects, Friedel pairs were merged; the absolute configuration was assigned on the basis of the known configuration of the starting material. All H atoms were placed in idealized positions (C—H = 0.93–0.98 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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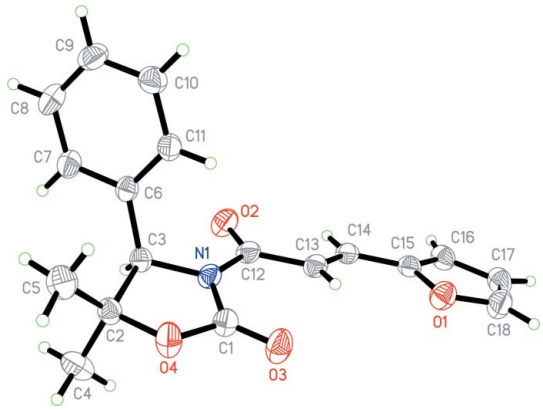

Figure 1
Molecular structure of (I), showing 30% displacement ellipoids (arbitrary spheres for the H atoms).

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