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6-*p*-Tolyl-2,2′-bipyridinyl-4-carboxylic acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.143
Data-to-parameter ratio = 15.9

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

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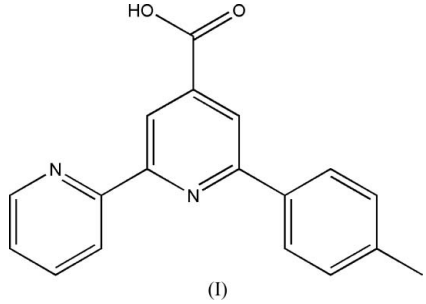
The title compound $C_{18}H_{14}N_2O_2$, forms centrosymmetric dimers *via* intermolecular O—H···N hydrogen bonds, with an O···N distance of 2.688 (3)Å and an O—H···N angle of 163°.

Comment

Hydrogen-bonding studies on pyridine carboxylic acid derivatives have received considerable attention due to the various interaction modes available (Crispini *et al.*, 2002). The most common packing motif is based on the formation of an intermolecular O—H···N hydrogen bond between the carboxyl group and the pyridine N atom of a second molecule. In such systems, the hydrogen bonding usually results in the formation of a chain (Blackburn *et al.*, 1996; Dobson *et al.*, 1998). However, in 2,6-diphenylpyridine-4-carboxylic acid (Crispini *et al.*, 2002), hydrogen bonding occurs only between carboxylic acid groups, leading to the formation of centrosymmetric dimers. In the title compound, (I), the carboxylic acid group forms a hydrogen bond with the N atom of a second molecule, forming a cyclic hydrogen-bonded $R_2^2(16)$ dimer (Bernstein *et al.*, 1995), with O2···N1^{i} = 2.688 (3) Å, O2—H2 = 0.82 Å, H2···N1^{i} = 1.89 Å and O2—H2···N1^{i} = 163° [symmetry code: (i) $-x+1, -y+2, -z$]. Weaker C—H···O interactions augment this hydrogen bond. All other bond distances and angles fall within normal ranges.



(I)

Experimental

The title compound, (I), was prepared as described in our previous paper (Cao *et al.*, 2004). Crystals suitable for X-ray diffraction analysis were recrystallized from methanol.

Crystal data

$C_{18}H_{14}N_2O_2$
M_r = 290.31
Monoclinic, $P2_1/n$
a = 14.699 (3) Å
b = 3.9680 (8) Å
c = 24.914 (5) Å
β = 105.67 (3)°
V = 1399.1 (5) Å^3
Z = 4
D_x = 1.378 Mg m^{-3}
Mo *Kα* radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Bruker APEX-II diffractometer	3208 independent reflections
φ and ω scans	1093 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.096$
13472 measured reflections	$\theta_{max} = 27.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.143$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
$S = 0.79$	$\Delta\rho_{min} = -0.20$ e Å^{-3}
3208 reflections	Extinction correction: *SHELXL97*
202 parameters	Extinction coefficient: 0.0121 (17)
H-atom parameters constrained	

H atoms were positioned geometrically (C—H = 0.93–0.96, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C,O)

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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, 2005); software used to prepare material for publication: *SHELXTL*.

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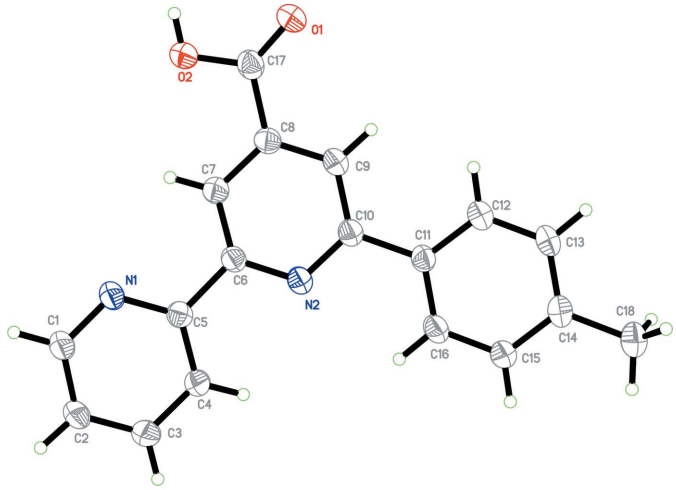

Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

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