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3-Cyano-6-(4-methoxyphenyl)-2(1*H*)-pyridone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.063
wR factor = 0.201
Data-to-parameter ratio = 15.5

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

The structure of the title compound, $C_{13}H_{10}N_2O_2$, comprises a twisted molecule with a dihedral angle of 37.81 (9)°. In the solid state, the molecules exist as typical 2(1*H*)-pyridone dimers *via* a hydrogen-bonding interaction from the N—H group to the O atom.

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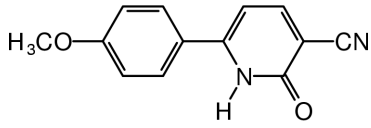
Comment

The structure of the title compound, (I), comprises a twisted molecule with a dihedral angle of 37.81 (9)°. In the solid state, the molecules exist as typical 2(1*H*)-pyridone dimers *via* a hydrogen-bonding interaction from the N—H group to the O atom. Molecules are also arranged head-to-tail with a C—H···N close contact from one of the methoxy H atoms to the cyano N atom.



(I)

Experimental

The title compound was obtained from Key Organics Ltd. Crystals were grown from an ethanol solution.

Crystal data

$C_{13}H_{10}N_2O_2$
M_r = 226.23
Monoclinic, $P2_1/n$
a = 10.6650 (7) Å
b = 9.8140 (8) Å
c = 11.1544 (12) Å
β = 108.833 (3)°
V = 1104.99 (17) Å^3
Z = 4
D_x = 1.360 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1832 reflections
θ = 1.0–27.5°
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colourless
0.30 × 0.10 × 0.03 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.972, T_{max} = 0.997
4925 measured reflections
2460 independent reflections
906 reflections with $I > 2\sigma(I)$
R_{int} = 0.094
θ_{max} = 27.4°
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 12$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.201
S = 0.90
2460 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0831P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

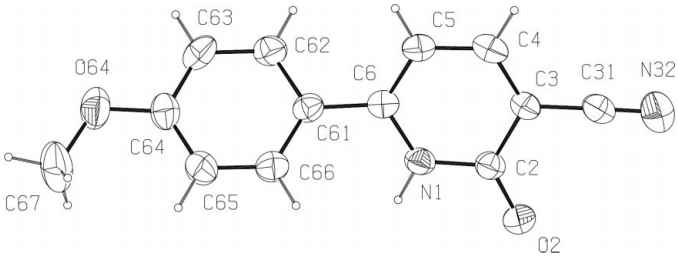


Figure 1
The molecular configuration and atom-numbering scheme, showing 50% probability ellipsoids.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.92 (4)	1.88 (4)	2.797 (4)	172 (3)
C4—H4···O2^{ii}	0.93	2.53	3.368 (4)	149
C67—H672···N32^{iii}	0.96	2.53	3.445 (5)	160

Symmetry codes: (i) $1-x,-y,1-z$; (ii) $\frac{3}{2}-x,y-\frac{1}{2},\frac{3}{2}-z$; (iii) $x-\frac{3}{2},-\frac{1}{2}-y,z-\frac{1}{2}$.

All H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.93 (Ar—H) and 0.96 Å (CH_3), except for the N—H atom, which was located in a difference syntheses and refined freely.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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