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4-(1,3-Benzodioxol-5-yl)-2-oxo-1,2,5,6-tetrahydrobenzo[*h*]quinoline-3-carbonitrile

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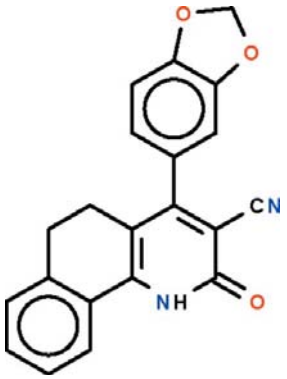
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.100; data-to-parameter ratio = 13.6.

In the molecule of the title compound, $C_{21}H_{14}N_2O_3$, the tetrahydrobenzo[*h*]quinoline fused-ring system is buckled owing to the ethylene $-CH_2CH_2-$ fragment, the benzene ring and the pyridine ring being twisted by 24.3 (1)°. The ring of the benzodioxol system is bent away from the pyridine ring by 61.4 (1)° in order to avoid crowding the cyanide substituent. Two molecules are linked by a pair of N—H···O hydrogen bonds to form a centrosymmetric dimer.

Related literature

For background to the anticancer properties of this class of compounds, see: Rostom *et al.* (2011).



Experimental

Crystal data

$C_{21}H_{14}N_2O_3$
M_r = 342.34
Monoclinic, $P2_1/n$
a = 7.6586 (3) Å
b = 16.5858 (5) Å
c = 13.3220 (6) Å
β = 104.164 (4)°
V = 1640.77 (11) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.802, T_{max} = 0.963
6078 measured reflections
3241 independent reflections
2962 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
S = 1.02
3241 reflections
239 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.93 (2)	1.85 (2)	2.778 (1)	175 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5293).

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