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

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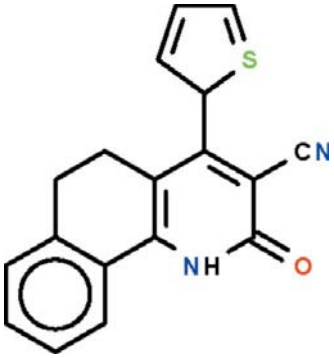
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.035; wR factor = 0.098; data-to-parameter ratio = 12.7.

In the molecule of the title compound, $C_{18}H_{12}N_2OS$, 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 16.0 (1)°. The 4-substituted aromatic ring is bent away from the pyridine ring by 59.5 (2)° (for the major disordered thienyl component) in order to avoid crowding the cyanide substituent. In the crystal, two molecules are linked by a pair of N—H···O hydrogen bonds to form a centrosymmetric dimer. The thienyl ring is disordered over two sites in a 72.7 (2):27.3 ratio.

Related literature

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



Experimental

Crystal data

$C_{18}H_{12}N_2OS$
M_r = 304.36
Triclinic, $P\overline{1}$
a = 6.9952 (3) Å
b = 9.1809 (4) Å
c = 11.1837 (5) Å
α = 93.990 (4)°
β = 95.293 (4)°
γ = 100.903 (4)°
V = 699.48 (5) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 2.07 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.575, T_{max} = 0.682
5795 measured reflections
2740 independent reflections
2600 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.098
S = 1.07
2740 reflections
216 parameters
19 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 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}	0.89 (1)	1.97 (1)	2.851 (1)	173 (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: XU5294).

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