Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Amino-1-(2*H*-1,3-benzodioxol-5-yl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile

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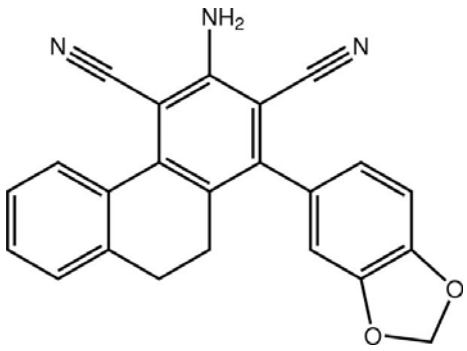
Received 16 August 2011; accepted 17 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.065; wR factor = 0.167; data-to-parameter ratio = 14.5.

In the title compound, $C_{23}H_{15}N_3O_2$, significant deviations from planarity are evidenced in the values of the dihedral angles formed between the amino-benzene ring and the benzene rings of the 1,3-benzodioxole [65.38 (12)°] and 1,2-dihydronaphthalene [26.27 (14)°] residues; the dioxole ring has an envelope conformation with the methylene-C being the flap atom. The amino-H atoms form hydrogen bonds to one of the dioxole-O atoms and to one of the cyano-N atoms to generate a two-dimensional array with a zigzag topology that stacks along the $(\bar{1}\ 0\ 2)$ plane.

Related literature

For background to the biological activity of related compounds, see: Aly *et al.* (1991); Al-Saadi *et al.* (2005); Rostom *et al.* (2011). For ring conformational analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{23}H_{15}N_3O_2$
M_r = 365.38
Monoclinic, $P2_1/c$
a = 8.9280 (6) Å
b = 22.4518 (13) Å
c = 8.9473 (6) Å
β = 109.058 (7)°
V = 1695.18 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.25 × 0.25 × 0.05 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.776, T_{max} = 1.000
9604 measured reflections
3775 independent reflections
2570 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.167
S = 1.02
3775 reflections
261 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O1^{i}	0.88 (1)	2.40 (2)	3.231 (3)	157 (3)
N2—H2···N1^{ii}	0.88 (1)	2.37 (2)	3.188 (3)	156 (3)

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

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: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2463).

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