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3-Amino-1-(4-methoxyphenyl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile

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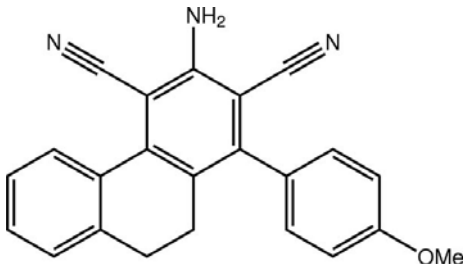
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.116; data-to-parameter ratio = 15.4.

In the title compound, $C_{23}H_{17}N_3O$, significant deviations from planarity are evidenced. This is quantified in the dihedral angles formed between the central amino-benzene ring and the benzene rings of the methoxybenzene [67.93 (8)°] and 1,2-dihydronaphthalene [28.27 (8)°] residues. In the crystal the amino-H atoms form hydrogen bonds to the methoxy-O atom and to one of the cyano-N atoms to generate a two-dimensional array with a zigzag topology that stacks along the $(\bar{1}\,\bar{1}\,1)$ 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). For a related structure, see: Asiri *et al.* (2011).



Experimental

Crystal data

$C_{23}H_{17}N_3O$
M_r = 351.40
Monoclinic, $P2_1/c$
a = 9.0212 (4) Å
b = 22.1475 (8) Å
c = 9.3114 (4) Å
β = 110.410 (5)°
V = 1743.60 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 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} = 0.714, T_{max} = 1.000
8688 measured reflections
3890 independent reflections
2953 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.116
S = 1.04
3890 reflections
252 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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}	0.89 (1)	2.21 (1)	3.0307 (19)	154 (2)
N2—H2···N1^{ii}	0.88 (1)	2.33 (1)	3.115 (2)	149 (2)

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5084).

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