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 = 0.048; wR = 0.116; data-to-parameter ratio = 15.4.

In the title compound, C23H17N3O, 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-dihyronaphthalene [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 (1 1 0) 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](image)

Crystal data

C23H17N3O

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) Å³

Z = 4

Mo Kα radiation

μ = 0.08 mm⁻¹

T = 100 K

0.25 × 0.25 × 0.05 mm

Table 1

Hydrogen-bond geometry (Å, °).

D–H···A D–H H···A D–A D–H···A

N2–H1 ···O1' 0.88 (1) 2.21 (1) 3.037 (19) 154 (2)

N2–H2 ···N1a 0.88 (1) 2.33 (1) 3.155 (2) 149 (2)

Symmetry codes: (i) x, −y + 1, z; (ii) −x + 1, −y, −z.

Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector

Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2010)

8688 measured reflections

2953 reflections with I > 2σ(I)

R_int = 0.030

Refinement

R[F² > 2σ(F²)] = 0.048

wR(F²) = 0.116

S = 1.04

3890 reflections

252 parameters

2 restraints

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

References


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