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

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In the title compound, C22H14BrN3, the fused-ring system is buckled owing to the ethylene linkage in the central ring; the two flanking aromatic rings are twisted by 25.9 (1)°/C14 relative to each other. The phenyl ring is twisted by 77.0 (1)/C14 relative to the amino- and cyano-bearing aromatic ring. In the crystal, adjacent molecules are linked by two N–H···N hydrogen bonds, generating a zigzag chain along [101].

Related literature

For two related compounds, see: Asiri et al. (2011a,b).

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Experimental

Crystal data

C22H14BrN3

Mr = 480.27

Monoclinic, Cc

b = 16.2557 (3) Å

c = 9.7945 (4) Å

β = 127.546 (6)°

V = 1738.07 (17) Å3

Z = 4

Cu Kα radiation

μ = 3.29 mm−1

T = 100 K

0.20 × 0.20 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector

2976 measured reflections

Absorption correction: multi-scan

2195 independent reflections

(CrysAlis PRO; Agilent, 2010)

2187 reflections with I > 2σ(I)

Tmin = 0.559, Tmax = 0.559

Refinement

H atoms treated by a mixture of independent and constrained refinement

Δρmax = 0.22 e Å−3

Δρmin = −0.61 e Å−3

Absolute structure: Flack (Flack, 1983), 482 Friedel pairs

Flack parameter: −0.024 (14)

Table 1

Hydrogen-bond geometry (Å, °).

D—H···A

D—H

H···A

D···A

D—H···A

N2—H2···N1i

0.93 (3)

2.23 (3)

3.097 (3)

155 (3)

N2—H2···N3ii

0.88 (4)

2.54 (4)

3.307 (3)

147 (3)

Symmetry codes: (i) x, −y + 1, z; (ii) 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: BT5646).

References


