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

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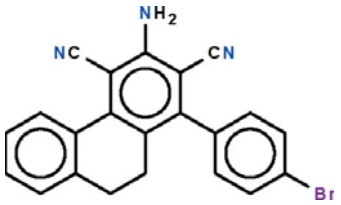
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.021; wR factor = 0.056; data-to-parameter ratio = 9.0.

In the title compound, $C_{22}H_{14}BrN_3$, 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) ° with respect to each other. The phenyl ring is twisted by 77.0 (1)° 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.* (2011*a*,*b*).



Experimental

Crystal data

$C_{22}H_{14}BrN_3$
M_r = 400.27
Monoclinic, *Cc*
a = 13.7683 (5) Å
b = 16.2557 (3) Å
c = 9.7945 (4) Å
β = 127.546 (6)°
V = 1738.07 (17) Å^3
Z = 4
Cu $K\alpha$ 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
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.559, T_{max} = 0.559
2976 measured reflections
2195 independent reflections
2187 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.056
S = 1.08
2195 reflections
243 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −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—H1···N1^{i}	0.93 (3)	2.23 (3)	3.097 (3)	155 (3)
N2—H2···N3^{ii}	0.88 (4)	2.54 (4)	3.307 (3)	147 (3)

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

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: *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).

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