

1-(4-Aminophenyl)-3-(3-bromophenyl)prop-2-en-1-one

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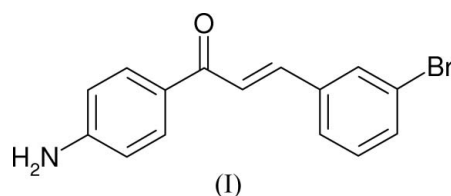
Key indicators

Single-crystal X-ray study
T = 273 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
R factor = 0.030
wR factor = 0.088
Data-to-parameter ratio = 31.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title molecule, $\text{C}_{15}\text{H}_{12}\text{BrNO}$, is approximately planar and the dihedral angle between the two aromatic rings is $9.6 (1)^\circ$. The crystal packing reveals that the molecules translated by one unit cell along the *a*-axis direction are linked into a chain by intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions. The screw-related molecules of adjacent chains are linked *via* $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds into a sheet-like structure parallel to the *ab* plane.

Comment

Chalcones (1,3-diarylpropen-1-ones) and their heterocyclic analogues possess a number of biological attributes and some of these have been reviewed. The antibacterial, fungistatic and fungicidal properties of these compounds have been reviewed by Opletalova (2000) and Opletalova & Sedivy (1999). The cytotoxic, anticancer, chemopreventative, mutagenic, antimicrobial, antiviral, antiprotozoal and insecticidal activities and enzyme-inhibitory properties of a variety of chalcones have also been reviewed (Dimmock *et al.*, 1999). Photo-cross-linkable polymers containing the chalcone group act as negative photo-resist materials used in a wide variety of applications (Balaji *et al.*, 2003). Chalcones are also used in designing effective second-order non-linear optical materials (Zhao *et al.*, 2000). The structure determination of the title compound, (I), was undertaken as part of our study of chalcones.



Bond lengths and angles in (I) are comparable with those reported for related structures (Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005). The short $\text{H5}\cdots\text{H8}$ (2.24 Å) contact causes the bond angles $\text{C5}-\text{C6}-\text{C7}$ [$123.07 (14)^\circ$] and $\text{C6}-\text{C7}-\text{C8}$ [$126.76 (14)^\circ$] to deviate significantly from 120° . Also, the short $\text{H8}\cdots\text{H11}$ (2.08 Å) contact results in a slight widening of the $\text{C9}-\text{C10}-\text{C11}$ angle to $122.97 (15)^\circ$. The sum of the angles around atom N1 is 349.7° and the deviation of atom N1 from the $\text{C13}/\text{H1A}/\text{H1B}$ plane is $0.19 (2) \text{ \AA}$, indicating its pyramidal nature.

The molecule of (I) (Fig. 1) is approximately planar. The enone fragment of the molecule containing atoms C7, C8, C9

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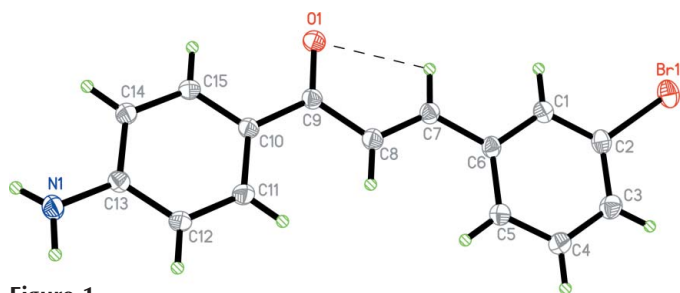


Figure 1

The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

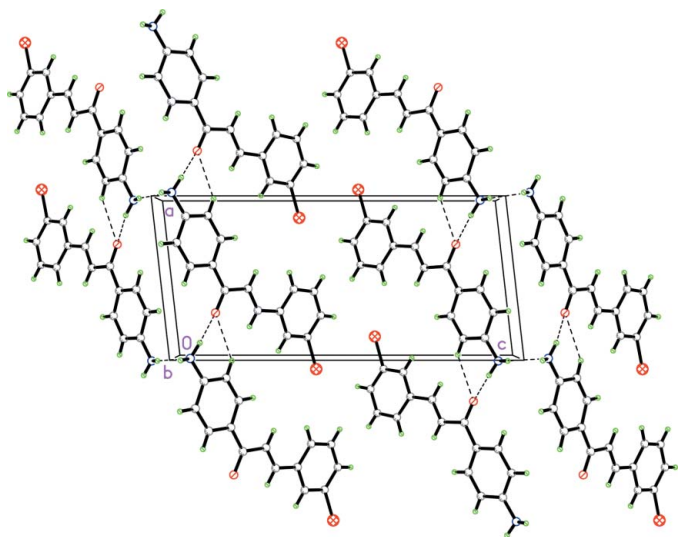


Figure 2

View of the hydrogen-bonded (dashed lines) sheets of (I).

and O1 is planar within ± 0.022 (2) Å. This plane makes dihedral angles of 3.1 (1) and 7.1 (1)°, respectively, with the C1–C6 and C10–C15 benzene rings. The dihedral angle between the benzene rings is 9.6 (1)°. The H atoms attached to C7 and C8 are *trans* to each other.

The weak intramolecular C7–H7···O1 interaction generates an *S*(5) ring motif. In the crystal structure, the molecules translated by one unit cell along the *a*-axis direction are linked by N1–H1A···O1ⁱ and C12–H12···O1ⁱ [symmetry code: (i) 1 + *x*, *y*, *z*] hydrogen-bonding interactions to form a chain (Table 1). These interactions together constitute a pair of bifurcated acceptor bonds, generating an *R*₂¹(6) motif (Bernstein *et al.*, 1995). The screw-related molecules of adjacent chains are linked *via* N1–H1B···N1ⁱⁱ [symmetry code: (ii) 2 – *x*, $\frac{1}{2}$ + *y*, –*z*] hydrogen bonds into a sheet-like structure parallel to the *ab* plane (Fig. 2).

Experimental

Compound (I) was obtained by the Claisen–Schmidt condensation of 4-aminoacetophenone (5.4 g, 0.04 mol) and 3-bromobenzaldehyde (7.4 g, 0.04 mol) in a 20% solution of NaOH and ethanol at 273 K over a period of 24 h. The product was isolated by neutralizing the reaction mixture with dilute hydrochloric acid. The crude product was recrystallized from ethanol.

Crystal data

C₁₅H₁₂BrNO
M_r = 302.17
 Monoclinic, *P*2₁
a = 8.0012 (2) Å
b = 4.6257 (1) Å
c = 17.1148 (5) Å
 β = 96.413 (1)°
V = 629.47 (3) Å³
Z = 2

D_x = 1.594 Mg m^{−3}
 Mo *K*α radiation
 Cell parameters from 6184 reflections
 θ = 2.6–37.8°
 μ = 3.25 mm^{−1}
T = 273 (2) K
 Block, colourless
 0.45 × 0.40 × 0.15 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
T_{min} = 0.324, *T_{max}* = 0.640
 9718 measured reflections

5338 independent reflections
 4831 reflections with *I* > 2σ(*I*)
R_{int} = 0.023
 θ_{max} = 38.2°
h = −13 → 13
k = −7 → 8
l = −27 → 27

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.030
wR (*F*²) = 0.088
S = 1.09
 5338 reflections
 171 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.36 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983),
 1968 Friedel pairs
 Flack parameter: 0.008 (6)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1A···O1 ⁱ	0.89 (2)	2.11 (3)	2.943 (2)	155 (3)
N1–H1B···N1 ⁱⁱ	0.89 (2)	2.33 (2)	3.157 (2)	155 (2)
C7–H7···O1	0.93	2.45	2.789 (2)	102
C12–H12···O1 ⁱ	0.93	2.49	3.241 (2)	138

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

Amino H atoms were located in a difference Fourier map and both positional and isotropic displacement parameters were refined, with an N–H distance restraint of 0.90 (1) Å. The C-bound H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C–H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C). The highest residual electron-density peak is located 0.76 Å from atom Br1.

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: SAINT (Bruker, 2005); program(s) used to solve structure: SHELXTL (Sheldrick, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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