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## Key indicators

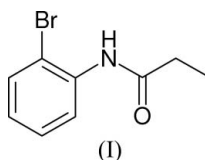
Single-crystal X-ray study  
 $T = 120\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.027  
 $wR$  factor = 0.065  
Data-to-parameter ratio = 18.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*N*-(2-Bromophenyl)propionamideThe title compound,  $\text{C}_9\text{H}_{10}\text{BrNO}$ , possesses normal geometrical parameters. The crystal packing is influenced by an  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond.

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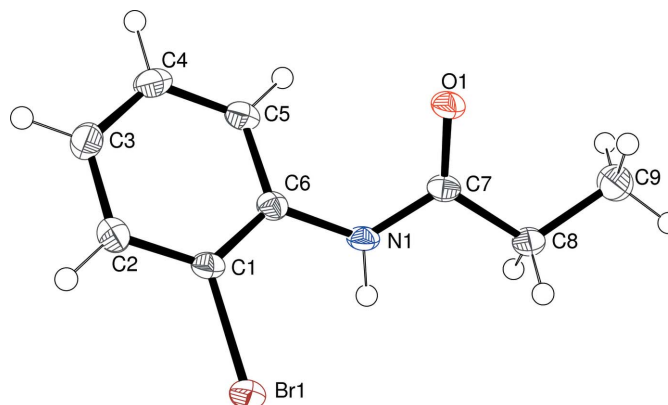
Online 14 September 2005

## Comment

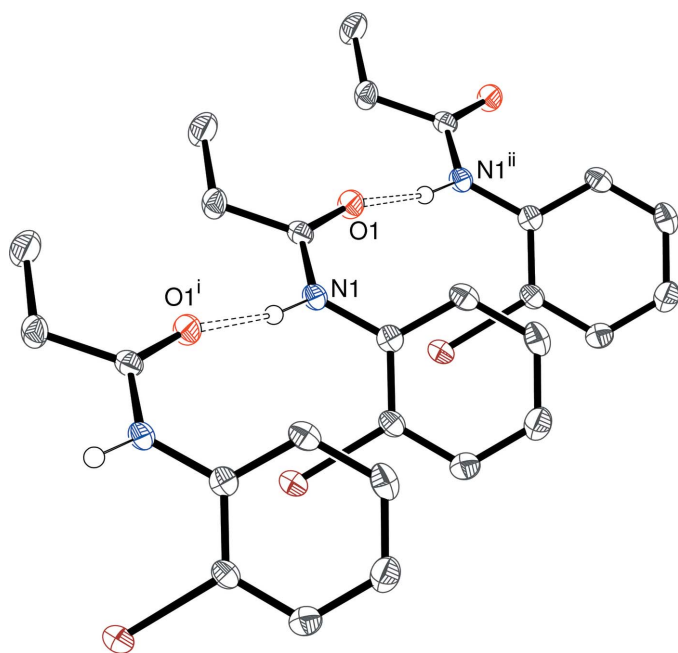
The title compound, (I) (Fig. 1), was prepared as part of our ongoing studies of acetanilide derivatives (Ronaldson *et al.*, 2005).

The dihedral angle between the mean planes of the benzene ring (atoms C1–C6) and the N1/O1/C7/C8 side chain is  $40.92(10)^\circ$ . This is very similar to the value [ $42.75(14)^\circ$ ] in *N*-(2-bromophenyl)acetamide, (II) (Ronaldson *et al.*, 2005). The bond angle sum about N1 in (I) is  $360.0^\circ$ , indicating that this atom is  $sp^2$  hybridized. The C6–N1 distance of  $1.416(3)\text{ \AA}$  in (I) is almost identical to the equivalent distance [ $1.418(4)\text{ \AA}$ ] in (II). All the other geometrical parameters for (I) lie within their expected ranges (Allen *et al.*, 1995).

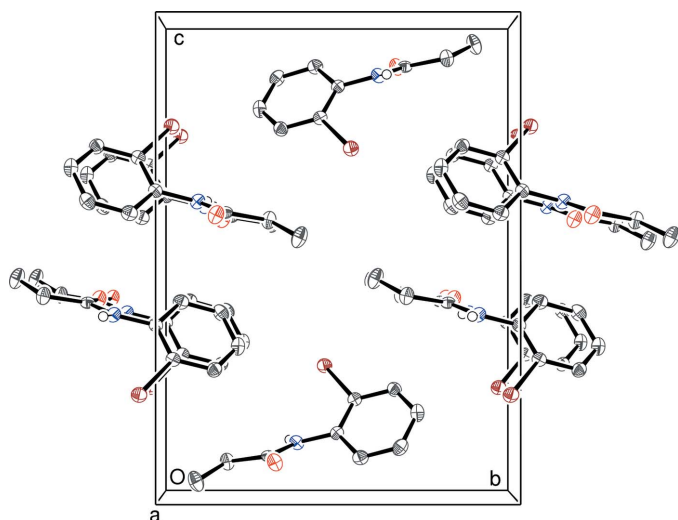
The crystal packing in (I) is influenced by an  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond (Table 1 and Fig. 2) that links the molecules into chains propagating in the  $[100]$  direction. There are no  $\pi-\pi$  interactions in (I). The unit-cell packing is shown in Fig. 3; (I) is essentially isostructural (same space group, similar unit-cell parameters) with (II), except that the unit cell for (I) is slightly expanded in the  $c$ -axis direction to accommodate the more bulky terminal ethyl moiety.



**Figure 1**  
View of (I), shown with 50% displacement ellipsoids. H atoms are drawn as small spheres of arbitrary radius.



**Figure 2**  
Detail of (I), showing how N—H...O hydrogen bonds (dashed lines) link molecules into a chain. The view direction is perpendicular to the mean plane of the benzene ring of the central molecule, showing that no  $\pi$ – $\pi$  stacking occurs. All H atoms except H1 have been omitted for clarity. [Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $x + 1, y, z$ .]



**Figure 3**  
The packing in (I), viewed down [010], with all H atoms except H1 omitted for clarity.

## Experimental

2-Bromoaniline (3.44 g, 20.0 mmol) was added to a solution of propionyl chloride (2.22 g, 24.0 mmol) and DIPEA (*N,N*-diisopropylethylamine) (3.12 g, 24.0 mmol) in dry tetrahydrofuran (20 ml) at 273 K. The reaction was monitored by thin-layer chromatography and, when complete, the mixture was diluted with water (20 ml) and the product was extracted with EtOAc (3  $\times$  20 ml). The organic phase was washed with water (2  $\times$  20 ml) and brine (20 ml) then dried over  $MgSO_4$  and evaporated under reduced pressure to

yield the crude product which was recrystallized from  $CH_2Cl_2$  to give 4.31 g (95% yield) of (I) as colourless needles. M.p. 360–362 K;  $R_F = 0.19$  [hexane/EtOAc (10:1)];  $\nu_{max}$  (KBr disc)/ $cm^{-1}$ : 3277 (NH), 2971–2932 (C—H), 1655 (C=O), 1573 (Ar C=C);  $\delta_H$  (250 MHz,  $CDCl_3$ ) 1.27 (3H, t,  $J = 7.5$  Hz,  $CH_3$ ), 2.46 (2H, q,  $J = 7.5$  Hz,  $CH_2$ ), 6.95 (1H, t,  $J = 7.5$  Hz, Ar—H), 7.29 (1H, t,  $J = 8.0$  Hz, Ar—H), 7.51 (1H, d,  $J = 8.0$  Hz, Ar—H), 8.35 (1H, d,  $J = 7.5$  Hz, Ar—H);  $\delta_C$  ( $CDCl_3$ ) 9.6 ( $CH_3$ ), 31.1 (—CO— $CH_2$ —), 113.2, 121.9, 125.0, 128.4, 132.2 and 135.7 (Ar—C), 172.0 (C=O).  $[M+H]^+$  226.994,  $C_9H_{10}^{79}BrNO$  requires 226.995.

## Crystal data

$C_9H_{10}BrNO$	$D_x = 1.658$ Mg m $^{-3}$
$M_r = 228.09$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2165 reflections
$a = 4.8701$ (1) Å	$\theta = 2.9$ – $27.5^\circ$
$b = 11.8048$ (4) Å	$\mu = 4.45$ mm $^{-1}$
$c = 15.9296$ (5) Å	$T = 120$ (2) K
$\beta = 93.964$ (2) $^\circ$	Needle, colourless
$V = 913.61$ (5) Å $^3$	$0.36 \times 0.05 \times 0.02$ mm
$Z = 4$	

## Data collection

Nonius KappaCCD diffractometer	1822 reflections with $I > 2\sigma(I)$
$\omega$ and $\varphi$ scans	$R_{int} = 0.043$
Absorption correction: multi-scan	$\theta_{max} = 27.5^\circ$
( <i>SADABS</i> ; Bruker, 2003)	$h = -6 \rightarrow 6$
$T_{min} = 0.297$ , $T_{max} = 0.916$	$k = -15 \rightarrow 15$
13742 measured reflections	$l = -20 \rightarrow 20$
2092 independent reflections	

## Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 0.9463P]$
$R[F^2 > 2\sigma(F^2)] = 0.027$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.065$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.38$ e Å $^{-3}$
2092 reflections	$\Delta\rho_{min} = -0.37$ e Å $^{-3}$
114 parameters	Extinction correction: <i>SHELXL97</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0039 (9)

**Table 1**  
Hydrogen-bond geometry (Å,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O1^i$	0.85 (3)	2.06 (3)	2.889 (2)	164 (2)

Symmetry code: (i)  $x - 1, y, z$ .

All C-bound H atoms were placed in idealized positions (C—H = 0.95–0.99 Å) and refined as riding on their carriers with the constraint  $U_{iso}(H) = 1.2U_{eq}(C)$  or  $U_{iso}(H) = 1.5U_{eq}(\text{methyl C})$  applied. The methyl group was allowed to rotate about the C9—C8 bond as a rigid group. The N-bound H atom was located in a difference map and its position was freely refined with the constraint  $U_{iso}(H) = 1.2U_{eq}(N)$ .

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997), and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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