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## Structure Reports

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# N-(4-Isopropoxyphenyl)acetamide

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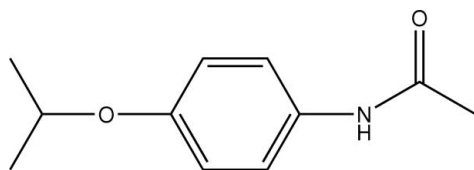
Received 31 March 2009; accepted 3 April 2009

 Key indicators: single-crystal X-ray study;  $T = 294$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.068;  $wR$  factor = 0.202; data-to-parameter ratio = 16.0.

In the molecule of the title compound,  $\text{C}_{11}\text{H}_{15}\text{NO}_2$ , the planar acetamide unit [maximum deviation of  $0.0014$  (6) Å] is oriented at a dihedral angle of  $19.68$  (4)° with respect to the aromatic ring. An intramolecular  $\text{C}-\text{H}\cdots\text{O}$  interaction results in the formation of a six-membered ring. In the crystal structure, intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into chains along the  $a$  axis

## Related literature

For general background, see: Knesl *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

 $\text{C}_{11}\text{H}_{15}\text{NO}_2$   
 $M_r = 193.24$ 

 Orthorhombic,  $Pbca$   
 $a = 9.3010$  (19) Å

 $b = 7.6490$  (15) Å  
 $c = 31.394$  (6) Å  
 $V = 2233.5$  (8) Å<sup>3</sup>  
 $Z = 8$ 

 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 294$  K  
 $0.30 \times 0.10 \times 0.10$  mm

### Data collection

 Enraf–Nonius CAD-4  
 diffractometer  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{\min} = 0.977$ ,  $T_{\max} = 0.992$   
 2026 measured reflections

 2026 independent reflections  
 1099 reflections with  $I > 2\sigma(I)$   
 3 standard reflections  
 frequency: 120 min  
 intensity decay: 1%

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.068$   
 $wR(F^2) = 0.202$   
 $S = 1.01$   
 2026 reflections

 127 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N}-\text{H}0\text{A}\cdots\text{O}2^i$	0.86	2.01	2.869 (3)	175
$\text{C}6-\text{H}6\text{A}\cdots\text{O}2$	0.93	2.34	2.892 (4)	118

 Symmetry code: (i)  $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ .

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2659).

## References

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**supplementary materials**

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## *N*-(4-Isopropoxyphenyl)acetamide

M. Zhang, R.-Z. Lu, L.-N. Han, W.-B. Wei and H.-B. Wang

### Comment

As part of our ongoing studies on tandutinib (Knesl *et al.*, 2006), we report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (C4-C9) is, of course, planar. The B (O2/N/C10/C11) moiety is also planar with a maximum deviation of -0.0014 (6) Å for C10 atom, and it is oriented with respect to ring A at a dihedral angle of 19.68 (4)°. Intramolecular C-H...O interaction (Table 1) results in the formation of a six-membered ring C (O2/N/C6/C7/C10/H6A), having twisted conformation.

In the crystal structure, intermolecular N-H...O hydrogen bonds (Table 1) link the molecules into chains along the *a* axis, in which they may be effective in the stabilization of the structure.

### Experimental

For the preparation of the title compound, *N*-(4-hydroxyphenyl)acetamide (50 mmol), 2-bromopropane (75 mmol) and potassium hydroxide (100 mmol) were mixed with ethanol (60 ml), and then the mixture was heated to reflux. Reaction progress was monitored by TLC. After ethanol removed in vacuo and filtration, the title compound was obtained (yield; 83.2%, m.p. 403 K). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate solution.

### Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å (for NH) and C-H = 0.93, 0.98 and 0.96 Å for aromatic, methine and methyl H, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C,N})$ , where  $x = 1.5$  for methyl H and  $x = 1.2$  for all other H atoms.

### Figures

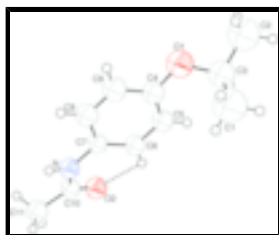


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Hydrogen bond is shown as dashed line.

## N-(4-isopropoxyphenyl)acetamide

### Crystal data

$C_{11}H_{15}NO_2$

$M_r = 193.24$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 9.3010$  (19) Å

$b = 7.6490$  (15) Å

$c = 31.394$  (6) Å

$V = 2233.5$  (8) Å<sup>3</sup>

$Z = 8$

$F_{000} = 832$

$D_x = 1.149$  Mg m<sup>-3</sup>

Melting point: 403 K

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 25 reflections

$\theta = 9\text{--}12^\circ$

$\mu = 0.08$  mm<sup>-1</sup>

$T = 294$  K

Block, colorless

$0.30 \times 0.10 \times 0.10$  mm

### Data collection

Enraf–Nonius CAD-4  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294$  K

$\omega/2\theta$  scans

Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)

$T_{\min} = 0.977$ ,  $T_{\max} = 0.992$

2026 measured reflections

2026 independent reflections

1099 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.0000$

$\theta_{\max} = 25.3^\circ$

$\theta_{\min} = 1.3^\circ$

$h = 0 \rightarrow 11$

$k = 0 \rightarrow 9$

$l = 0 \rightarrow 37$

3 standard reflections

every 120 min

intensity decay: 1%

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.068$

$wR(F^2) = 0.202$

$S = 1.01$

2026 reflections

127 parameters

Primary atom site location: structure-invariant direct  
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring  
sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.26$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>

Extinction correction: none

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and goodness of fit S are based on  $F^2$ , conventional R-factors R are based on F, with F set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\text{sigma}(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N	0.5437 (3)	0.2110 (3)	0.52353 (8)	0.0516 (7)
H0A	0.4609	0.2564	0.5183	0.062*
O1	0.5722 (3)	-0.0692 (3)	0.68713 (7)	0.0834 (8)
O2	0.7614 (2)	0.1579 (3)	0.49473 (7)	0.0665 (7)
C1	0.5187 (7)	-0.3739 (7)	0.67643 (15)	0.128 (2)
H1A	0.5192	-0.3613	0.6460	0.192*
H1B	0.4231	-0.3546	0.6870	0.192*
H1C	0.5494	-0.4897	0.6839	0.192*
C2	0.6254 (7)	-0.2587 (7)	0.74329 (13)	0.1163 (17)
H2A	0.6915	-0.1733	0.7542	0.175*
H2B	0.6577	-0.3737	0.7510	0.175*
H2C	0.5318	-0.2385	0.7552	0.175*
C3	0.6181 (5)	-0.2437 (6)	0.69566 (12)	0.0810 (12)
H3A	0.7146	-0.2607	0.6838	0.097*
C4	0.5728 (4)	-0.0080 (4)	0.64580 (11)	0.0602 (9)
C5	0.6698 (3)	-0.0586 (4)	0.61512 (10)	0.0589 (9)
H5A	0.7396	-0.1415	0.6215	0.071*
C6	0.6637 (3)	0.0134 (4)	0.57479 (10)	0.0543 (8)
H6A	0.7297	-0.0221	0.5543	0.065*
C7	0.5608 (3)	0.1378 (4)	0.56435 (9)	0.0470 (8)
C8	0.4652 (4)	0.1886 (5)	0.59609 (12)	0.0631 (10)
H8A	0.3955	0.2722	0.5900	0.076*
C9	0.4712 (4)	0.1183 (5)	0.63610 (11)	0.0680 (10)
H9A	0.4069	0.1555	0.6569	0.082*
C10	0.6390 (3)	0.2191 (4)	0.49183 (10)	0.0515 (8)
C11	0.5892 (4)	0.3070 (5)	0.45170 (11)	0.0638 (10)
H11A	0.6652	0.3047	0.4310	0.096*
H11B	0.5638	0.4260	0.4578	0.096*
H11C	0.5069	0.2464	0.4406	0.096*

## supplementary materials

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### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N	0.0428 (13)	0.0549 (16)	0.0572 (16)	0.0014 (12)	-0.0018 (11)	0.0035 (13)
O1	0.119 (2)	0.0703 (17)	0.0608 (16)	0.0233 (16)	0.0052 (14)	0.0019 (13)
O2	0.0471 (13)	0.0715 (16)	0.0808 (16)	0.0047 (12)	0.0103 (12)	0.0115 (12)
C1	0.198 (6)	0.092 (4)	0.094 (4)	-0.034 (4)	0.005 (4)	0.003 (3)
C2	0.168 (5)	0.107 (4)	0.074 (3)	0.024 (4)	0.001 (3)	0.022 (3)
C3	0.096 (3)	0.069 (2)	0.078 (3)	0.014 (2)	0.008 (2)	0.011 (2)
C4	0.076 (2)	0.0508 (19)	0.054 (2)	0.0052 (19)	-0.0027 (17)	-0.0050 (16)
C5	0.061 (2)	0.051 (2)	0.065 (2)	0.0133 (17)	-0.0040 (16)	0.0000 (17)
C6	0.0534 (18)	0.0518 (19)	0.058 (2)	0.0022 (16)	0.0051 (15)	-0.0014 (16)
C7	0.0428 (15)	0.0439 (17)	0.0543 (19)	-0.0027 (14)	-0.0004 (13)	-0.0027 (14)
C8	0.062 (2)	0.057 (2)	0.071 (2)	0.0136 (17)	0.0049 (17)	0.0004 (18)
C9	0.076 (2)	0.064 (2)	0.063 (2)	0.017 (2)	0.0114 (17)	-0.0049 (19)
C10	0.0486 (17)	0.0420 (18)	0.064 (2)	-0.0084 (15)	0.0008 (15)	-0.0044 (15)
C11	0.061 (2)	0.063 (2)	0.067 (2)	-0.0106 (18)	-0.0042 (16)	0.0080 (18)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

N—C10	1.334 (4)	C4—C5	1.375 (4)
N—C7	1.407 (4)	C4—C9	1.385 (4)
N—H0A	0.8600	C5—C6	1.382 (4)
O1—C4	1.379 (4)	C5—H5A	0.9300
O1—C3	1.427 (5)	C6—C7	1.389 (4)
O2—C10	1.234 (4)	C6—H6A	0.9300
C1—C3	1.487 (6)	C7—C8	1.391 (4)
C1—H1A	0.9600	C8—C9	1.367 (5)
C1—H1B	0.9600	C8—H8A	0.9300
C1—H1C	0.9600	C9—H9A	0.9300
C2—C3	1.501 (5)	C10—C11	1.501 (4)
C2—H2A	0.9600	C11—H11A	0.9600
C2—H2B	0.9600	C11—H11B	0.9600
C2—H2C	0.9600	C11—H11C	0.9600
C3—H3A	0.9800		
C10—N—C7	128.5 (3)	C4—C5—C6	120.2 (3)
C10—N—H0A	115.7	C4—C5—H5A	119.9
C7—N—H0A	115.7	C6—C5—H5A	119.9
C4—O1—C3	119.5 (3)	C5—C6—C7	121.2 (3)
C3—C1—H1A	109.5	C5—C6—H6A	119.4
C3—C1—H1B	109.5	C7—C6—H6A	119.4
H1A—C1—H1B	109.5	C6—C7—C8	117.6 (3)
C3—C1—H1C	109.5	C6—C7—N	124.4 (3)
H1A—C1—H1C	109.5	C8—C7—N	118.0 (3)
H1B—C1—H1C	109.5	C9—C8—C7	121.5 (3)
C3—C2—H2A	109.5	C9—C8—H8A	119.3
C3—C2—H2B	109.5	C7—C8—H8A	119.3

H2A—C2—H2B	109.5	C8—C9—C4	120.3 (3)
C3—C2—H2C	109.5	C8—C9—H9A	119.9
H2A—C2—H2C	109.5	C4—C9—H9A	119.9
H2B—C2—H2C	109.5	O2—C10—N	122.7 (3)
O1—C3—C1	111.3 (4)	O2—C10—C11	121.1 (3)
O1—C3—C2	105.8 (3)	N—C10—C11	116.2 (3)
C1—C3—C2	112.4 (4)	C10—C11—H11A	109.5
O1—C3—H3A	109.1	C10—C11—H11B	109.5
C1—C3—H3A	109.1	H11A—C11—H11B	109.5
C2—C3—H3A	109.1	C10—C11—H11C	109.5
C5—C4—O1	124.5 (3)	H11A—C11—H11C	109.5
C5—C4—C9	119.3 (3)	H11B—C11—H11C	109.5
O1—C4—C9	116.1 (3)		
C4—O1—C3—C1	-65.9 (5)	C10—N—C7—C6	-21.2 (5)
C4—O1—C3—C2	171.7 (4)	C10—N—C7—C8	161.2 (3)
C3—O1—C4—C5	-32.2 (5)	C6—C7—C8—C9	-0.4 (5)
C3—O1—C4—C9	150.6 (4)	N—C7—C8—C9	177.4 (3)
O1—C4—C5—C6	-178.5 (3)	C7—C8—C9—C4	-0.8 (5)
C9—C4—C5—C6	-1.3 (5)	C5—C4—C9—C8	1.7 (5)
C4—C5—C6—C7	0.2 (5)	O1—C4—C9—C8	179.0 (3)
C5—C6—C7—C8	0.7 (5)	C7—N—C10—O2	0.6 (5)
C5—C6—C7—N	-176.9 (3)	C7—N—C10—C11	-179.7 (3)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N—H0A $\cdots$ O2 <sup>i</sup>	0.86	2.01	2.869 (3)	175
C6—H6A $\cdots$ O2	0.93	2.34	2.892 (4)	118

Symmetry codes: (i)  $x-1/2, -y+1/2, -z+1$ .

Fig. 1

