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N-[2-(4-Bromophenoxy)ethyl]acetamide

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The crystal structure of the title compound, $C_{10}H_{12}BrNO_2$, is stabilized mainly through intermolecular N—H···O hydrogen bonds.

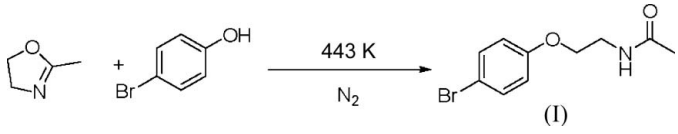
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.039
wR factor = 0.090
Data-to-parameter ratio = 16.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

2-Phenoxyethanamine is a starting material for the preparation of the antidepressant drug nefazodone (Madding, 1986). The title compound, (I), which can be hydrolyzed to 2-(4-bromophenoxy)ethanamine, was obtained in order to prepare new analogous compounds.



(I)

The molecular geometry in (I) is normal (Allen *et al.*, 1987). The crystal structure is stabilized mainly through intermolecular N—H···O hydrogen bonds (Table 1), resulting in $C(4)$ chains (Etter, 1990).

Experimental

A mixture of 4-bromophenol (17.3 g, 0.10 mol) and 2-methyl-4,5-dihydrooxazole (1.2 g, 0.12 mol) was slowly heated to reflux under nitrogen and refluxed for 7 h, monitored by thin-layer chromatography. On completion, the excess 2-methyl-4,5-dihydrooxazole was recovered by distillation, the residue was cooled to room temperature and 10% NaOH solution (50 ml) was added. The product was filtered off and purifed by column chromatography. The title compound (20 mg) was dissolved in methanol (15 ml) and after 15 d colourless blocks of (I) were recovered.

Crystal data

$C_{10}H_{12}BrNO_2$
M_r = 258.12
Monoclinic, $P2_1$
a = 4.9957 (16) Å
b = 9.340 (3) Å
c = 11.700 (4) Å
β = 95.882 (6)°
V = 543.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.76 mm^{-1}
T = 294 (2) K
0.28 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.419, T_{max} = 0.520
(expected range = 0.380–0.472)
3109 measured reflections
2099 independent reflections
1445 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.090
S = 0.98
2099 reflections
131 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Absolute structure: Flack (1983), with 915 Friedel pairs
Flack parameter: 0.006 (16)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.83 (4)	2.07 (5)	2.905 (5)	176 (5)

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

The N-bound H atom was located in a difference map and its position was freely refined, with U_{iso}(H) = 1.2U_{eq}(N). The C-bound H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined in a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

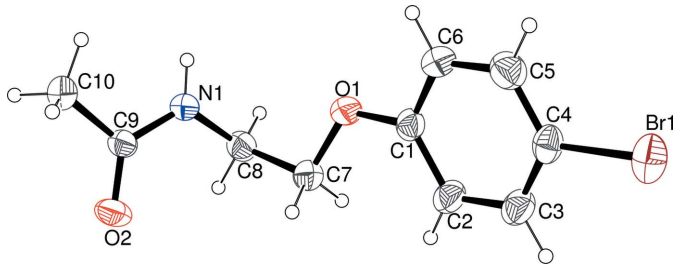


Figure 1
The molecular structure of (I), drawn with 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

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