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3-(2-Bromophenyl)-*N*-phenyloxirane-2-carboxamide

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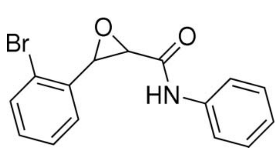
Key indicators: single-crystal X-ray study; *T* = 295 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.028; *wR* factor = 0.069; data-to-parameter ratio = 15.3.

In the molecule of the title compound, $C_{15}H_{12}BrNO_2$, the two benzene rings adopt a *syn* configuration with respect to the epoxy ring; the dihedral angles between the epoxy ring and the two benzene rings are 59.90 (13) and 68.01 (12)°. Intermolecular N—H···O and C—H···O hydrogen bonding is present in the crystal structure.

Related literature

For epoxide-containing compounds used as building blocks in synthesis, see: Flisak *et al.* (1993); Watanabe *et al.* (1998); Zhu & Espenson (1995). For related structures, see: He (2009); He & Chen (2009).



Experimental

Crystal data

$C_{15}H_{12}BrNO_2$
M_r = 318.17
Orthorhombic, $P2_12_12_1$
a = 6.71700 (10) Å
b = 10.0370 (2) Å
c = 20.4287 (3) Å
V = 1377.27 (4) Å^3
Z = 4
Cu *K*α radiation
μ = 4.05 mm^{-1}
T = 295 K
0.40 × 0.40 × 0.36 mm

Data collection

Oxford Diffraction Gemini S Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis Pro*; Oxford Diffraction, 2009)
T_{min} = 0.294, T_{max} = 0.324
17721 measured reflections
2701 independent reflections
2675 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.069
S = 1.01
2701 reflections
177 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Absolute structure: Flack (1983), 1104 Friedel pairs
Flack parameter: −0.008 (18)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.79 (3)	2.22 (3)	2.971 (2)	161 (2)
C15—H15···O1^{ii}	0.93	2.59	3.442 (3)	153

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

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2009); 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: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The diffraction data were collected at The Centre for Testing and Analysis, Sichuan University. We acknowledge financial support from China West Normal University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2664).

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supporting information

Acta Cryst. (2009). E**65**, o2999 [doi:10.1107/S1600536809045929]

3-(2-Bromophenyl)-*N*-phenyloxirane-2-carboxamide

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S1. Comment

Epoxides are important intermediates in organic synthesis. Glycidic esters and amides are particularly useful as they can be further transformed to key intermediates of several pharmaceutical products (Flisak *et al.* 1993; Watanabe *et al.* 1998). The Darzens reaction, is one of the most powerful methodologies for the synthesis of α, β-epoxy carbonyl and related compounds (Zhu & Espenson, 1995). We report herein the crystal structure of the title compound.

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles in (I) are normal. In the molecule, the two phenyl ring adopts a *cis* configuration about the epoxides ring. The dihedral angle between the C1—C6 and C10—C15 is 77.05 (7)°, O1/C7/C8 epoxide ring makes dihedral angles of 59.90 (13)° and 68.01 (12)° with C6 and C15 phenyl ring, respectively, which is similar to that found in a related structure (He & Chen, 2009). The crystal packing is stabilized by N—H···0 and C—H···0 hydrogen bonding (Table 1).

S2. Experimental

2-Chloro-*N*-phenylacetamide (0.17 g, 1.0 mmol) and potassium hydroxide (0.112 g, 2.0 mmol) were dissolved in acetonitrile (2 ml). To the solution was added 2-bromophenylaldehyde (0.15 g, 1.0 mmol) at 298 K, the solution was stirred for 60 min and removal of solvent under reduced pressure, the residue was purified through column chromatography. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature for 1 d.

S3. Refinement

Imine H atom was located in a difference Fourier map and refined isotropically. The carbon-bound hydrogen atoms were placed in calculated positions, with C—H = 0.93–0.98 Å, and refined using a riding model with U_{iso}(H) =1.2U_{eq}(C).

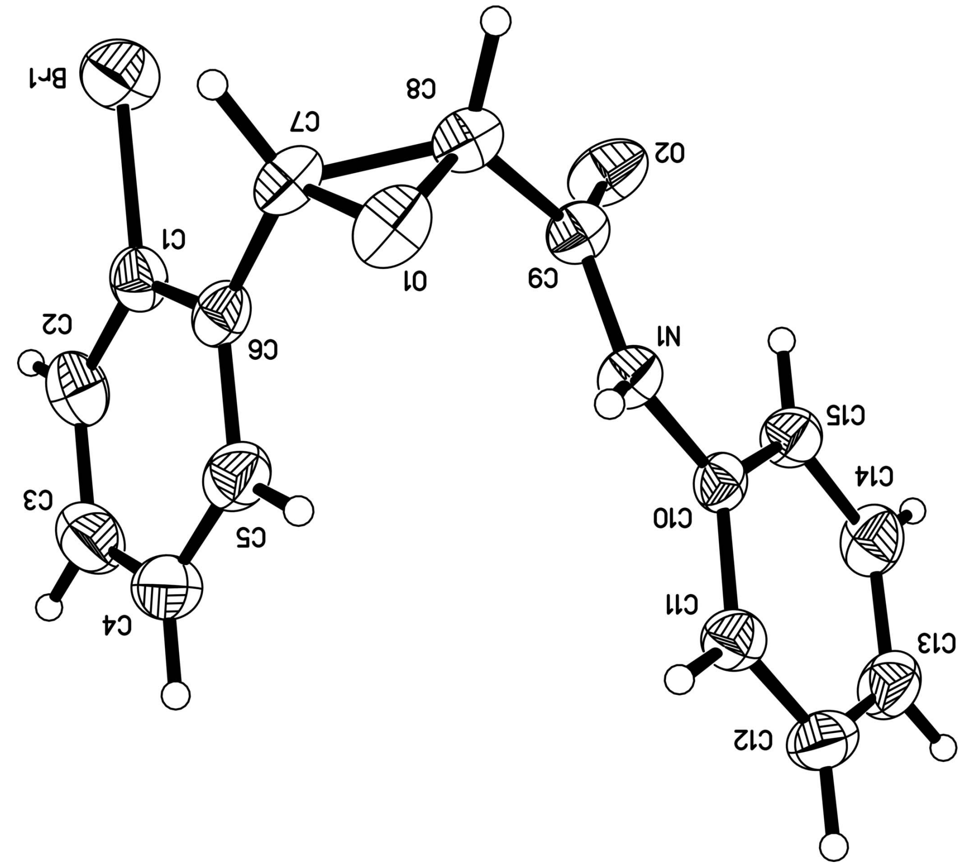

Figure 1

The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

3-(2-Bromophenyl)-*N*-phenyloxirane-2-carboxamide

Crystal data

$C_{15}H_{12}BrNO_2$
M_r = 318.17
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 6.7170 (1) Å
b = 10.0370 (2) Å
c = 20.4287 (3) Å
V = 1377.27 (4) Å^3
Z = 4

F(000) = 640
D_x = 1.534 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 15647 reflections
θ = 2.2–72.1°
μ = 4.05 mm^{-1}
T = 295 K
Block, colorless
0.40 × 0.40 × 0.36 mm

Data collection

Oxford Diffraction Gemini S Ultra diffractometer
Radiation source: Enhance Ultra (Cu) X-ray Source
Mirror monochromator
Detector resolution: 15.9149 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)

T_{min} = 0.294, T_{max} = 0.324
17721 measured reflections
2701 independent reflections
2675 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 72.3°, θ_{min} = 4.3°
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 12$
$l = -24 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.069$
$S = 1.01$
2701 reflections
177 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 0.5235P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0074 (5)
Absolute structure: Flack (1983), 1104 Friedel pairs
Absolute structure parameter: −0.008 (18)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	−0.14003 (5)	0.63054 (3)	0.557209 (16)	0.07563 (15)
O1	−0.1933 (3)	0.23595 (16)	0.66346 (9)	0.0567 (4)
O2	−0.0059 (3)	0.50889 (16)	0.76057 (10)	0.0637 (5)
N1	0.1077 (3)	0.29560 (18)	0.75313 (9)	0.0437 (4)
C5	0.1656 (4)	0.2794 (3)	0.59008 (13)	0.0582 (6)
H5	0.1480	0.2015	0.6140	0.070*
C6	0.0186 (3)	0.3772 (2)	0.59138 (10)	0.0470 (5)
C15	0.3410 (4)	0.4080 (2)	0.82806 (11)	0.0520 (5)
H15	0.2588	0.4823	0.8314	0.062*
C9	−0.0201 (3)	0.3947 (2)	0.74074 (11)	0.0440 (4)
C8	−0.1951 (3)	0.3600 (2)	0.69813 (11)	0.0467 (5)
H8	−0.3253	0.3893	0.7143	0.056*
C10	0.2882 (3)	0.3016 (2)	0.78857 (10)	0.0407 (4)
C7	−0.1724 (3)	0.3564 (2)	0.62606 (11)	0.0499 (5)
H7	−0.2912	0.3828	0.6014	0.060*
C11	0.4155 (3)	0.1931 (2)	0.78350 (11)	0.0494 (5)
H11	0.3828	0.1227	0.7559	0.059*
C1	0.0535 (4)	0.4931 (2)	0.55591 (11)	0.0502 (5)
C12	0.5905 (4)	0.1889 (3)	0.81914 (14)	0.0607 (6)
H12	0.6734	0.1149	0.8162	0.073*
C2	0.2261 (5)	0.5119 (3)	0.52052 (13)	0.0654 (7)
H2	0.2477	0.5908	0.4977	0.078*

C3	0.3657 (5)	0.4116 (3)	0.51958 (14)	0.0723 (7)
H3	0.4815	0.4227	0.4952	0.087*
C13	0.6420 (4)	0.2934 (3)	0.85879 (13)	0.0655 (7)
H13	0.7594	0.2905	0.8829	0.079*
C14	0.5199 (4)	0.4020 (3)	0.86281 (13)	0.0641 (7)
H14	0.5567	0.4734	0.8892	0.077*
C4	0.3375 (4)	0.2965 (3)	0.55369 (14)	0.0680 (7)
H4	0.4334	0.2297	0.5525	0.082*
H1	0.074 (3)	0.225 (3)	0.7406 (12)	0.037 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0896 (2)	0.05464 (17)	0.0827 (2)	0.01486 (15)	0.01432 (17)	0.01807 (14)
O1	0.0611 (10)	0.0400 (8)	0.0689 (10)	−0.0133 (7)	−0.0136 (8)	0.0087 (7)
O2	0.0677 (10)	0.0342 (8)	0.0891 (12)	0.0036 (8)	−0.0200 (10)	−0.0011 (8)
N1	0.0487 (10)	0.0311 (8)	0.0515 (9)	−0.0032 (8)	−0.0056 (8)	−0.0002 (7)
C5	0.0618 (15)	0.0547 (13)	0.0581 (13)	0.0042 (12)	−0.0126 (12)	−0.0037 (11)
C6	0.0500 (11)	0.0458 (11)	0.0453 (10)	−0.0031 (11)	−0.0122 (8)	−0.0024 (9)
C15	0.0584 (13)	0.0455 (11)	0.0520 (11)	0.0046 (10)	−0.0047 (11)	−0.0052 (9)
C9	0.0473 (10)	0.0332 (10)	0.0515 (11)	−0.0039 (8)	−0.0011 (9)	0.0071 (8)
C8	0.0418 (10)	0.0375 (10)	0.0609 (12)	−0.0063 (9)	−0.0036 (8)	0.0089 (10)
C10	0.0442 (10)	0.0386 (10)	0.0392 (9)	−0.0030 (8)	0.0020 (8)	0.0079 (8)
C7	0.0459 (11)	0.0448 (11)	0.0589 (12)	−0.0055 (10)	−0.0150 (9)	0.0106 (10)
C11	0.0517 (12)	0.0425 (11)	0.0541 (12)	0.0011 (9)	0.0042 (9)	0.0029 (9)
C1	0.0604 (12)	0.0462 (11)	0.0441 (10)	−0.0012 (9)	−0.0009 (10)	−0.0020 (10)
C12	0.0477 (12)	0.0615 (14)	0.0730 (16)	0.0100 (11)	0.0029 (11)	0.0138 (12)
C2	0.0782 (17)	0.0652 (16)	0.0528 (13)	−0.0086 (14)	0.0095 (12)	−0.0001 (12)
C3	0.0631 (16)	0.091 (2)	0.0629 (15)	−0.0026 (16)	0.0099 (14)	−0.0143 (14)
C13	0.0525 (13)	0.0838 (19)	0.0602 (13)	0.0019 (15)	−0.0100 (12)	0.0111 (13)
C14	0.0696 (16)	0.0679 (16)	0.0548 (13)	−0.0056 (14)	−0.0149 (12)	−0.0083 (12)
C4	0.0624 (15)	0.0748 (17)	0.0669 (15)	0.0141 (13)	−0.0095 (15)	−0.0156 (14)

Geometric parameters (Å, º)

Br1—C1	1.896 (2)	C8—H8	0.9800
O1—C8	1.433 (3)	C10—C11	1.388 (3)
O1—C7	1.437 (3)	C7—H7	0.9800
O2—C9	1.219 (3)	C11—C12	1.384 (4)
N1—C9	1.338 (3)	C11—H11	0.9300
N1—C10	1.414 (3)	C1—C2	1.380 (4)
N1—H1	0.78 (3)	C12—C13	1.370 (4)
C5—C4	1.384 (4)	C12—H12	0.9300
C5—C6	1.392 (3)	C2—C3	1.375 (5)
C5—H5	0.9300	C2—H2	0.9300
C6—C1	1.390 (3)	C3—C4	1.363 (5)
C6—C7	1.481 (3)	C3—H3	0.9300
C15—C10	1.385 (3)	C13—C14	1.366 (4)

C15—C14	1.397 (4)	C13—H13	0.9300
C15—H15	0.9300	C14—H14	0.9300
C9—C8	1.503 (3)	C4—H4	0.9300
C8—C7	1.481 (3)		

C8—O1—C7	62.11 (14)	O1—C7—H7	114.9
C9—N1—C10	127.97 (19)	C6—C7—H7	114.9
C9—N1—H1	115.1 (18)	C8—C7—H7	114.9
C10—N1—H1	116.8 (18)	C12—C11—C10	120.6 (2)
C4—C5—C6	121.0 (3)	C12—C11—H11	119.7
C4—C5—H5	119.5	C10—C11—H11	119.7
C6—C5—H5	119.5	C2—C1—C6	121.9 (2)
C1—C6—C5	117.4 (2)	C2—C1—Br1	118.96 (19)
C1—C6—C7	120.9 (2)	C6—C1—Br1	119.09 (17)
C5—C6—C7	121.7 (2)	C13—C12—C11	120.1 (2)
C10—C15—C14	118.9 (2)	C13—C12—H12	119.9
C10—C15—H15	120.6	C11—C12—H12	119.9
C14—C15—H15	120.6	C3—C2—C1	118.7 (3)
O2—C9—N1	125.9 (2)	C3—C2—H2	120.6
O2—C9—C8	118.1 (2)	C1—C2—H2	120.6
N1—C9—C8	116.05 (19)	C4—C3—C2	121.2 (3)
O1—C8—C7	59.09 (14)	C4—C3—H3	119.4
O1—C8—C9	118.74 (18)	C2—C3—H3	119.4
C7—C8—C9	120.07 (19)	C14—C13—C12	119.7 (2)
O1—C8—H8	115.7	C14—C13—H13	120.2
C7—C8—H8	115.7	C12—C13—H13	120.2
C9—C8—H8	115.7	C13—C14—C15	121.3 (2)
C15—C10—C11	119.4 (2)	C13—C14—H14	119.3
C15—C10—N1	123.5 (2)	C15—C14—H14	119.3
C11—C10—N1	117.1 (2)	C3—C4—C5	119.7 (3)
O1—C7—C6	117.2 (2)	C3—C4—H4	120.1
O1—C7—C8	58.80 (14)	C5—C4—H4	120.1
C6—C7—C8	124.15 (18)		

C4—C5—C6—C1	−1.3 (3)	C9—C8—C7—O1	107.5 (2)
C4—C5—C6—C7	175.4 (2)	O1—C8—C7—C6	−103.6 (2)
C10—N1—C9—O2	−3.1 (4)	C9—C8—C7—C6	3.9 (4)
C10—N1—C9—C8	176.5 (2)	C15—C10—C11—C12	2.1 (3)
C7—O1—C8—C9	−109.7 (2)	N1—C10—C11—C12	−176.9 (2)
O2—C9—C8—O1	167.2 (2)	C5—C6—C1—C2	0.1 (3)
N1—C9—C8—O1	−12.5 (3)	C7—C6—C1—C2	−176.7 (2)
O2—C9—C8—C7	98.3 (3)	C5—C6—C1—Br1	−178.98 (16)
N1—C9—C8—C7	−81.4 (3)	C7—C6—C1—Br1	4.2 (3)
C14—C15—C10—C11	−1.2 (3)	C10—C11—C12—C13	−1.4 (4)
C14—C15—C10—N1	177.8 (2)	C6—C1—C2—C3	1.1 (4)
C9—N1—C10—C15	14.1 (3)	Br1—C1—C2—C3	−179.8 (2)
C9—N1—C10—C11	−166.9 (2)	C1—C2—C3—C4	−1.2 (4)
C8—O1—C7—C6	115.3 (2)	C11—C12—C13—C14	−0.2 (4)

C1—C6—C7—O1	−177.83 (19)	C12—C13—C14—C15	1.1 (4)
C5—C6—C7—O1	5.5 (3)	C10—C15—C14—C13	−0.4 (4)
C1—C6—C7—C8	−108.6 (2)	C2—C3—C4—C5	0.0 (4)
C5—C6—C7—C8	74.7 (3)	C6—C5—C4—C3	1.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.79 (3)	2.22 (3)	2.971 (2)	161 (2)
C15—H15···O1^{ii}	0.93	2.59	3.442 (3)	153

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+3/2; (ii) −*x*, *y*+1/2, −*z*+3/2.