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# 1-{[2-(Bromomethyl)-2-(4-chlorophenyl)-1,3-dioxolan-4-yl]methyl}-1*H*-1,2,4-triazole

**Yue-Qin Yu,[a] Ai-Xiang Dong,[b] Xue-Mei Li,[b] Ping-Kai Ouyang[a] and Shu-Sheng Zhang[a]***

[a]College of Life Science and Pharmaceutical Engineering, Nanjing University of Technology, 210093 Nanjing, Jiangsu, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

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**Key indicators**

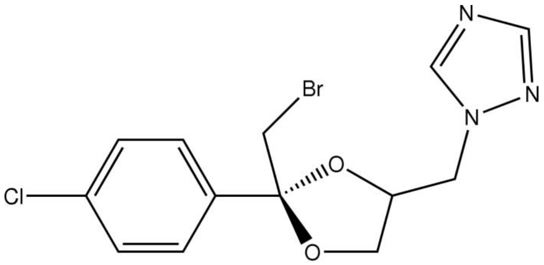
Single-crystal X-ray study
*T* = 293 K
Mean $\sigma$(C–C) = 0.003 Å
*R* factor = 0.030
*wR* factor = 0.079
Data-to-parameter ratio = 15.6

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

In the molecule of the title compound, $C_{13}H_{13}BrClN_3O_2$, the dioxolane ring adopts an envelope conformation. The benzene ring is almost perpendicular to the triazole ring, with a dihedral angle of 84.1 (1)°. The crystal packing is stabilized by C—H···O and C—H···N hydrogen bonds.

## Comment

Triazole compounds containing 1,3-dioxolane have the ability to prevent plant diseases (Chai, 1985). In the present study, a novel triazole compound, (I), containing 1,3-dioxolane, has been synthesized from cheap 3-chloropropane-1,2-diol instead of expensive pentane-1,2-diol.



(I)

The bond lengths and angles in (I) (Table 1) show normal values (Allen *et al.*, 1987). The dioxolane ring adopts an envelope conformation, with O1 as the flap atom The O1—C7—C4 angle is 112.1 (2)°, implying that the benzene ring attached to C7 is oriented away from the dioxolane ring. Atom Br1 is located as far away as possible with respect to the benzene ring, the C4—C7—C13—Br1 torsion angle being −176.7 (1)°. The benzene ring is almost perpendicular to the triazole ring, with a dihedral angle of 84.1 (1)°.

In the molecular structure of (I), there is an intramolecular C—H···O hydrogen bond (Table 2), forming a five-membered ring. In the crystal structure, molecules are linked by an intermolecular C—H···N hydrogen bond into a chain parallel to the *b* axis (Fig. 2). Another C—H···N interaction further links the chains into a three-dimensional framework.

## Experimental

Bromine (1.92 g, 24 mmol) was added dropwise to a solution of 4-chloroacetophenone (3.10 g, 20 mmol) in anhydrous diethyl ether (50 ml) in an ice-bath. The reaction was maintained for 6 h to give $\omega$-bromine-4-chloroacetophenone. Anhydrous 3-chloro-1,2-propane diol (3.33 g, 30 mmol), 1-butanol (10 ml) and toluene-*p*-sulfonic acid (0.1 g, 0.2 mmol) were then added. The reaction mixture was refluxed for 7 h and then cooled to room temperature. The organic layer was washed with saturated sodium bicarbonate solution and dried over anhydrous sodium sulfate. A white solid was obtained by recrystallization from methanol. A solution of this compound (7.82 g, 24 mmol) in dimethylformamide (15 ml) was added to a solution of sodium triazole (2.18 g, 24 mmol) and dried KI (0.5 g, 3 mmol) in dimethylformamide (50 ml). The mixture was heated to reflux for 5 h and then the solution was washed with water and extracted with chloroform. Single crystals of (I) were obtained by slow evaporation of a solution of the product in petroleum ether–ethyl acetate (3:1 *v*/*v*) at room temperature over a period of 3 d.

*Crystal data*

$C_{13}H_{13}BrClN_3O_2$
$M_r$ = 358.62
Monoclinic, $P2_1/c$
$a$ = 17.0510 (12) Å
$b$ = 7.6708 (6) Å
$c$ = 11.2732 (8) Å
$\beta$ = 101.419 (1)°
$V$ = 1445.29 (18) Å$^3$
$Z$ = 4
$D_x$ = 1.648 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 3.03 mm$^{-1}$
$T$ = 293 (2) K
Plate, colourless
0.35 × 0.25 × 0.08 mm

*Data collection*

Siemens SMART 1000 CCD area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.417, $T_{\max}$ = 0.793
8083 measured reflections
2828 independent reflections
2342 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.018
$\theta_{\max}$ = 26.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.079
$S$ = 1.04
2828 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.4373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.23 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Br1—C13 | 1.949 (2) | O2—C9 | 1.448 (3) |
| Cl1—C1 | 1.749 (2) | N1—N2 | 1.359 (3) |
| O1—C7 | 1.415 (2) | C7—C13 | 1.511 (3) |
| O1—C8 | 1.439 (3) | C8—C9 | 1.527 (3) |
| O2—C7 | 1.429 (2) | C9—C10 | 1.499 (3) |
| C7—O1—C8 | 105.32 (17) | O1—C7—C13 | 109.91 (18) |
| O1—C7—O2 | 105.92 (16) | O1—C7—C4 | 112.08 (17) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3*B*···O1 | 0.93 | 2.48 | 2.806 (3) | 100 |
| C10—H10*A*···N2$^{\rm i}$ | 0.97 | 2.57 | 3.340 (3) | 136 |
| C11—H11*A*···N3$^{\rm ii}$ | 0.93 | 2.56 | 3.262 (3) | 133 |

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

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

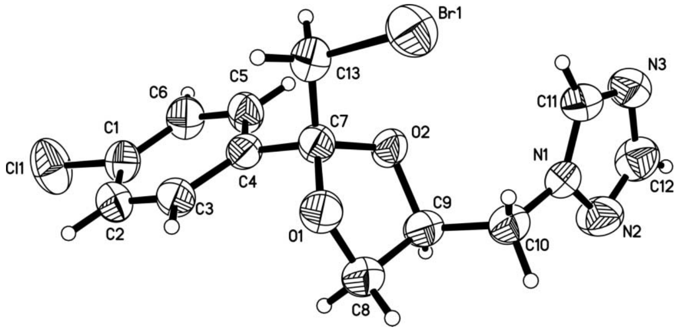


**Figure 1**
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

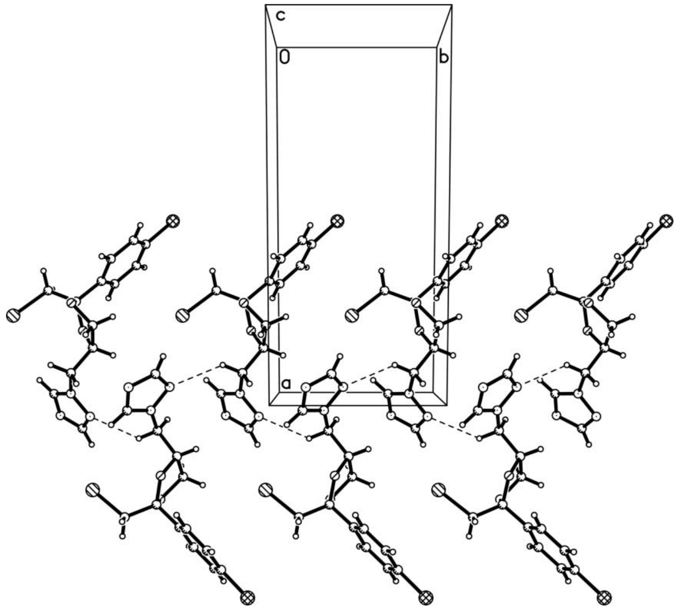


**Figure 2**
A partial packing diagram for (I), viewed down the *c* axis. C—H···N hydrogen bonds are indicated by dashed lines.

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