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# 3-(2*H*-Benzotriazol-2-yl)-1-(4-fluorophenyl)propan-1-one

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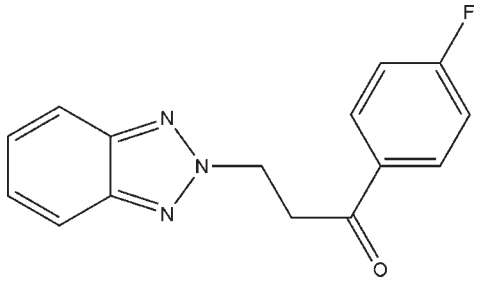
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.081; $wR$ factor = 0.210; data-to-parameter ratio = 6.9.

In the title compound, $C_{15}H_{12}FN_3O$, the benzotriazole ring system is essentially planar, with a maximum deviation from the least-squares plane of 0.016 (3) Å. The dihedral angle between this ring system and the fluoro-substituted benzene ring is 67.97 (2)°. The crystal structure is stabilized by weak intermolecular C—H···N interactions.

## Related literature

For applications of benzotriazole derivatives, see: Chen & Wu (2005). For standard bond distances, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{15}H_{12}FN_3O$
$M_r$ = 269.28
Monoclinic, $P2_1$
$a$ = 5.7858 (12) Å
$b$ = 5.6814 (11) Å
$c$ = 19.313 (4) Å
$\beta$ = 90.77 (3)°
$V$ = 634.8 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 293 K
0.20 × 0.18 × 0.10 mm

### Data collection

Bruker SMART CCD diffractometer
3943 measured reflections
1240 independent reflections
1122 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.135

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.081
$wR(F^2)$ = 0.210
$S$ = 1.07
1240 reflections
181 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14$B$···N1$^{i}$ | 0.97 | 2.58 | 3.511 (3) | 161 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5027).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Z.-Y. & Wu, M.-J. (2005). *Org. Lett.* **7**, 475–477.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2010). E**66**, o1124 [https://doi.org/10.1107/S1600536810013917]

## 3-(2*H*-Benzotriazol-2-yl)-1-(4-fluorophenyl)propan-1-one

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### S1. Comment

1*H*-Benzotriazole and its derivatives are an important class of compounds because they exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen & Wu., 2005). 1*H* and 2*H*-Benzotriazole are tautomers. We report here the synthesis and structure of the title compound, (I) (Fig. 1), as part of our ongoing studies on new benzotriazole compounds with potential bioactivity. All bond lengths (Allen *et al.*, 1987) and angles in (I) are within normal ranges. The benzotriazole ring system is essentially planar with a maximum deviation from the least squares plane of 0.016 (3)Å. The dihedral angle between this ring system and the fluro substituted benzene ring is 67.97 (2). The crystal structure is stabilized by weak intermolecular C—H···N interactions.

### S2. Experimental

To a solution of 1-(4-ethylphenyl)-3-(dimethylamino)propan-1-one (12.05 g, 0.05 mol) in water (25 ml) was added benzotriazole (7.1 g, 0.06 mol). The mixture was heated under reflux for 5 h. The solution was filtered,concentrated and purified by flash chromatography (silica gel,using petroleum ether-ethylacetate(4:1 *v*/*v*). to afford the title compound. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a ethanol solution over a period of 5 d.

### S3. Refinement

In the absence of significant anomalous dispersion effects the Friedel pairs were merged. All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C) .

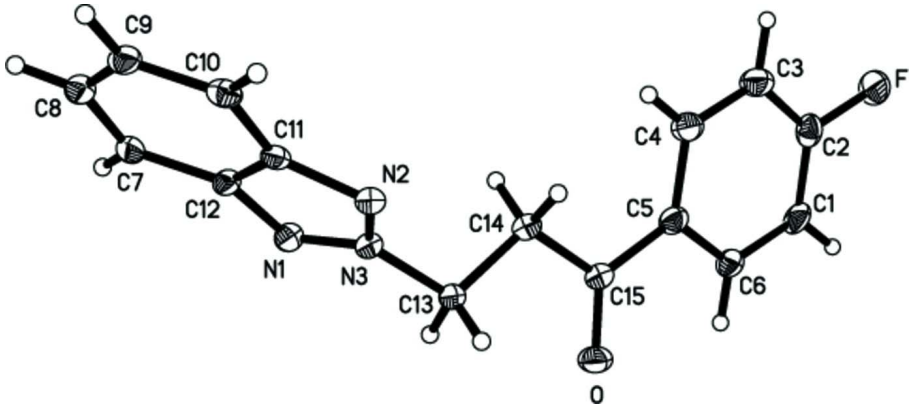


**Figure 1**

The molecular structure of (I), drawn with 30% probability ellipsoids.

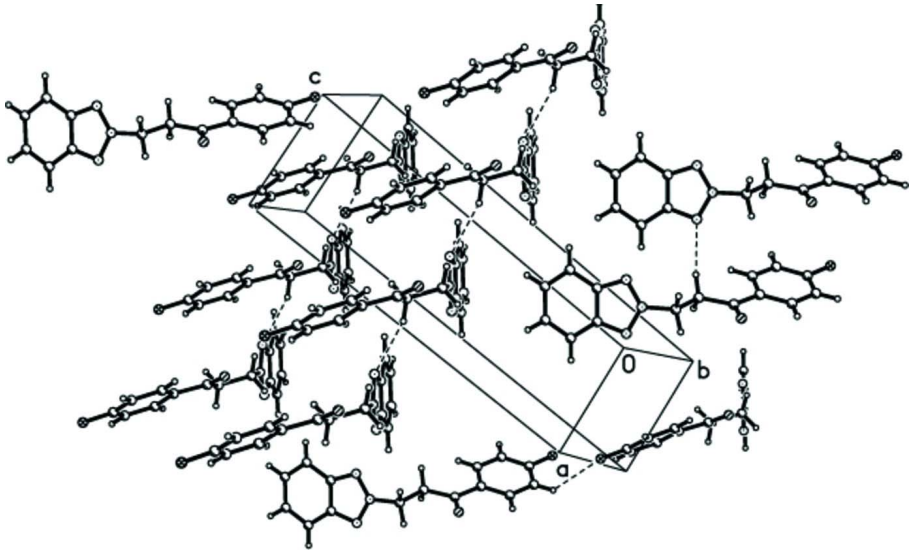


**Figure 2**

Part of the crystal structure of (I) showing hydrogen bonds as dashed lines.

### 3-(2*H*-Benzotriazol-2-yl)-1-(4-fluorophenyl)propan-1-one

*Crystal data*

$C_{15}H_{12}FN_3O$
$M_r = 269.28$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 5.7858\ (12)$ Å
$b = 5.6814\ (11)$ Å
$c = 19.313\ (4)$ Å
$\beta = 90.77\ (3)°$
$V = 634.8\ (2)$ Å$^3$
$Z = 2$
$F(000) = 280$
$D_x = 1.409$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1874 reflections
$\theta = 1.1–25.0°$
$\mu = 0.10$ mm$^{-1}$
$T = 293$ K
Block, colorless
0.20 × 0.18 × 0.10 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
3943 measured reflections
1240 independent reflections
1122 reflections with $I > 2\sigma(I)$
$R_{int} = 0.135$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.1°$
$h = -6\rightarrow6$
$k = -6\rightarrow6$
$l = -22\rightarrow20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.081$
$wR(F^2) = 0.210$
$S = 1.07$
1240 reflections
181 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.1432P)^2 + 0.1388P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.34$ e Å$^{-3}$

*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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F | 0.0574 (7) | 1.0117 (7) | 0.01386 (19) | 0.0505 (11) |
| O | 0.9115 (8) | 1.3049 (7) | 0.1980 (2) | 0.0434 (12) |
| N1 | 1.3671 (7) | 0.6871 (8) | 0.3093 (2) | 0.0278 (10) |
| N2 | 1.0658 (8) | 0.6958 (8) | 0.3810 (2) | 0.0300 (10) |
| N3 | 1.1720 (8) | 0.7892 (8) | 0.3293 (2) | 0.0265 (10) |
| C9 | 1.3499 (10) | 0.1759 (10) | 0.4572 (3) | 0.0316 (13) |
| H9A | 1.3402 | 0.0609 | 0.4913 | 0.038* |
| C15 | 0.8110 (10) | 1.1189 (10) | 0.1966 (3) | 0.0300 (13) |
| C14 | 0.8827 (10) | 0.9205 (9) | 0.2440 (3) | 0.0292 (12) |
| H14A | 0.9270 | 0.7856 | 0.2164 | 0.035* |
| H14B | 0.7524 | 0.8746 | 0.2720 | 0.035* |
| C12 | 1.3905 (9) | 0.5068 (10) | 0.3556 (3) | 0.0274 (12) |
| C5 | 0.6140 (11) | 1.0790 (10) | 0.1461 (3) | 0.0326 (13) |
| C13 | 1.0823 (9) | 0.9904 (10) | 0.2907 (3) | 0.0293 (12) |
| H13A | 1.2047 | 1.0571 | 0.2630 | 0.035* |
| H13B | 1.0315 | 1.1103 | 0.3229 | 0.035* |
| C11 | 1.2016 (9) | 0.5119 (10) | 0.4001 (3) | 0.0276 (12) |
| C2 | 0.2439 (10) | 1.0338 (10) | 0.0570 (3) | 0.0344 (14) |
| C6 | 0.5609 (10) | 1.2550 (10) | 0.0984 (3) | 0.0315 (13) |
| H6A | 0.6528 | 1.3891 | 0.0966 | 0.038* |
| C10 | 1.1818 (10) | 0.3418 (10) | 0.4533 (3) | 0.0285 (12) |
| H10A | 1.0595 | 0.3438 | 0.4841 | 0.034* |
| C8 | 1.5400 (10) | 0.1698 (10) | 0.4116 (3) | 0.0336 (13) |
| H8A | 1.6498 | 0.0512 | 0.4164 | 0.040* |
| C3 | 0.2883 (12) | 0.8551 (12) | 0.1038 (3) | 0.0416 (15) |
| H3A | 0.1945 | 0.7223 | 0.1050 | 0.050* |
| C4 | 0.4757 (11) | 0.8775 (10) | 0.1490 (3) | 0.0356 (14) |
| H4A | 0.5090 | 0.7594 | 0.1809 | 0.043* |
| C7 | 1.5654 (10) | 0.3346 (10) | 0.3607 (3) | 0.0309 (12) |
| H7A | 1.6910 | 0.3332 | 0.3311 | 0.037* |
| C1 | 0.3754 (11) | 1.2338 (10) | 0.0540 (3) | 0.0376 (15) |
| H1B | 0.3395 | 1.3526 | 0.0226 | 0.045* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F | 0.048 (2) | 0.046 (2) | 0.057 (2) | 0.0034 (19) | −0.0271 (17) | −0.0036 (19) |
| O | 0.048 (3) | 0.026 (2) | 0.056 (3) | −0.007 (2) | −0.019 (2) | 0.006 (2) |
| N1 | 0.027 (2) | 0.025 (2) | 0.031 (3) | 0.001 (2) | −0.0019 (17) | 0.0008 (19) |
| N2 | 0.027 (2) | 0.021 (2) | 0.042 (3) | −0.001 (2) | −0.0053 (18) | −0.002 (2) |
| N3 | 0.028 (2) | 0.020 (2) | 0.032 (3) | 0.0000 (18) | −0.0043 (18) | −0.0002 (19) |
| C9 | 0.040 (3) | 0.025 (3) | 0.029 (3) | −0.010 (3) | −0.012 (2) | 0.006 (2) |
| C15 | 0.030 (3) | 0.022 (3) | 0.037 (3) | 0.001 (2) | −0.004 (2) | −0.004 (2) |
| C14 | 0.033 (3) | 0.023 (3) | 0.032 (3) | 0.001 (2) | 0.000 (2) | −0.002 (2) |
| C12 | 0.030 (3) | 0.020 (2) | 0.032 (3) | −0.002 (2) | −0.010 (2) | 0.004 (2) |
| C5 | 0.038 (3) | 0.025 (3) | 0.035 (3) | 0.002 (2) | −0.004 (2) | −0.005 (2) |
| C13 | 0.028 (3) | 0.020 (2) | 0.040 (3) | 0.000 (2) | −0.011 (2) | −0.001 (2) |
| C11 | 0.028 (3) | 0.021 (2) | 0.034 (3) | −0.011 (2) | −0.009 (2) | 0.002 (2) |
| C2 | 0.032 (3) | 0.039 (3) | 0.031 (3) | 0.011 (3) | −0.008 (2) | −0.007 (3) |
| C6 | 0.035 (3) | 0.026 (3) | 0.034 (3) | 0.004 (2) | −0.005 (2) | 0.006 (2) |
| C10 | 0.032 (3) | 0.027 (3) | 0.026 (3) | −0.008 (2) | −0.0030 (19) | −0.001 (2) |
| C8 | 0.036 (3) | 0.027 (3) | 0.038 (3) | −0.004 (2) | −0.012 (2) | 0.001 (3) |
| C3 | 0.044 (4) | 0.030 (3) | 0.050 (4) | −0.007 (3) | −0.010 (3) | −0.002 (3) |
| C4 | 0.042 (3) | 0.030 (3) | 0.035 (3) | −0.003 (3) | −0.007 (2) | −0.001 (3) |
| C7 | 0.028 (3) | 0.024 (3) | 0.040 (3) | 0.000 (2) | −0.009 (2) | −0.006 (2) |
| C1 | 0.043 (4) | 0.025 (3) | 0.044 (4) | 0.010 (3) | −0.010 (3) | 0.009 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F—C2 | 1.360 (7) | C5—C6 | 1.390 (8) |
| O—C15 | 1.207 (7) | C5—C4 | 1.399 (9) |
| N1—N3 | 1.331 (7) | C13—H13A | 0.9700 |
| N1—C12 | 1.364 (7) | C13—H13B | 0.9700 |
| N2—N3 | 1.293 (7) | C11—C10 | 1.416 (8) |
| N2—C11 | 1.356 (7) | C2—C1 | 1.369 (9) |
| N3—C13 | 1.457 (7) | C2—C3 | 1.381 (9) |
| C9—C10 | 1.356 (8) | C6—C1 | 1.370 (9) |
| C9—C8 | 1.419 (9) | C6—H6A | 0.9300 |
| C9—H9A | 0.9300 | C10—H10A | 0.9300 |
| C15—C14 | 1.506 (7) | C8—C7 | 1.367 (9) |
| C15—C5 | 1.508 (7) | C8—H8A | 0.9300 |
| C14—C13 | 1.510 (7) | C3—C4 | 1.388 (9) |
| C14—H14A | 0.9700 | C3—H3A | 0.9300 |
| C14—H14B | 0.9700 | C4—H4A | 0.9300 |
| C12—C11 | 1.400 (8) | C7—H7A | 0.9300 |
| C12—C7 | 1.410 (8) | C1—H1B | 0.9300 |
| | | | |
| N3—N1—C12 | 102.4 (4) | H13A—C13—H13B | 108.0 |
| N3—N2—C11 | 104.3 (5) | N2—C11—C12 | 107.7 (5) |
| N2—N3—N1 | 117.3 (4) | N2—C11—C10 | 132.1 (5) |
| N2—N3—C13 | 123.2 (5) | C12—C11—C10 | 120.2 (5) |

| | | | |
|---|---|---|---|
| N1—N3—C13 | 119.4 (5) | F—C2—C1 | 119.2 (5) |
| C10—C9—C8 | 122.9 (5) | F—C2—C3 | 118.2 (5) |
| C10—C9—H9A | 118.5 | C1—C2—C3 | 122.6 (5) |
| C8—C9—H9A | 118.5 | C1—C6—C5 | 121.0 (5) |
| O—C15—C14 | 120.9 (5) | C1—C6—H6A | 119.5 |
| O—C15—C5 | 120.4 (5) | C5—C6—H6A | 119.5 |
| C14—C15—C5 | 118.7 (5) | C9—C10—C11 | 116.7 (5) |
| C15—C14—C13 | 111.6 (5) | C9—C10—H10A | 121.6 |
| C15—C14—H14A | 109.3 | C11—C10—H10A | 121.6 |
| C13—C14—H14A | 109.3 | C7—C8—C9 | 121.5 (5) |
| C15—C14—H14B | 109.3 | C7—C8—H8A | 119.3 |
| C13—C14—H14B | 109.3 | C9—C8—H8A | 119.3 |
| H14A—C14—H14B | 108.0 | C4—C3—C2 | 118.7 (6) |
| N1—C12—C11 | 108.4 (5) | C4—C3—H3A | 120.6 |
| N1—C12—C7 | 129.2 (5) | C2—C3—H3A | 120.6 |
| C11—C12—C7 | 122.4 (5) | C3—C4—C5 | 119.5 (6) |
| C6—C5—C4 | 119.6 (5) | C3—C4—H4A | 120.2 |
| C6—C5—C15 | 118.6 (5) | C5—C4—H4A | 120.2 |
| C4—C5—C15 | 121.7 (5) | C8—C7—C12 | 116.2 (6) |
| N3—C13—C14 | 111.3 (5) | C8—C7—H7A | 121.9 |
| N3—C13—H13A | 109.4 | C12—C7—H7A | 121.9 |
| C14—C13—H13A | 109.4 | C2—C1—C6 | 118.6 (5) |
| N3—C13—H13B | 109.4 | C2—C1—H1B | 120.7 |
| C14—C13—H13B | 109.4 | C6—C1—H1B | 120.7 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14*B*···N1$^{i}$ | 0.97 | 2.58 | 3.511 (3) | 161 |

Symmetry code: (i) *x*−1, *y*, *z*.