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3-(1*H*-1,2,4-Triazol-4-yl)phenol

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Key indicators

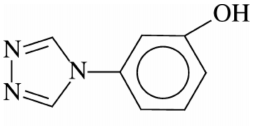
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.119
Data-to-parameter ratio = 11.9

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

In the structure of the title compound, $C_8H_7N_3O$, there are two molecules in the asymmetric unit. Intermolecular O—H···N hydrogen bonds link the molecules into two independent one-dimensional chains extending along the **c** direction.

Comment

Substituted 1,2,4-triazoles can be synthesized from different amines and diformylhydrazine. The triazole ring, having strong σ-donor and weak π-acceptor properties, potentially has two different coordination modes through three nitrogen-donor atoms coordinating to metal ions (Van Diemen *et al.*, 1991). Recent interest in substituted 1,2,4-triazoles has arisen in part from their transition metal complexes with intriguing structures and specific magnetic properties. Many metal complexes containing substituted 1,2,4-triazole have potential applications in molecular-based memory devices, displays and optical switches due to their spin crossover properties (Garcia *et al.*, 1997; Kahn & Martinez, 1998). In contrast to the extensively studied metal complexes with triazole acting as ligand, there are relatively few crystal structures of substituted 1,2,4-triazole. We report here the synthesis and structure of a new substituted 1,2,4-triazole, namely 3-(1*H*-1,2,4-triazol-4-yl)phenol, (I), which is isomeric with 4-(1*H*-1,2,4-triazol-1-yl)phenol (Foces-Foces *et al.*, 1999).



(I)

The crystal structure of (I) has two crystallographically independent molecules in the asymmetric unit. Corresponding bond lengths and angles in the two molecules are the same within experimental error. The only significant difference between the two independent molecules is in the dihedral

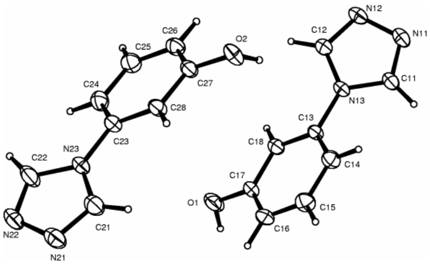


Figure 1
The molecular structure of the title compound, showing both independent molecules. Displacement ellipsoids are drawn at the 30% probability level.

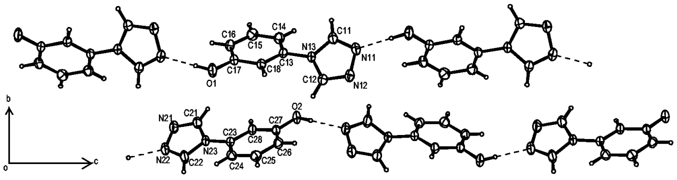


Figure 2
Independent hydrogen-bonded chains of the title compound, extending along the **c** direction. Hydrogen bonds are shown as dashed lines.

angles between the triazole and phenol rings, which are 22.9 (1) and 37.4 (1)°. C—N bond distances in (I) are in good agreement with those found in other substituted 1,2,4-triazole compounds (Foces-Foces *et al.*, 1999; Kunkeler *et al.*, 1996; Abramovitch *et al.*, 2001; Cai *et al.*, 1999; Palmer & Parsons, 1996; Chen *et al.*, 2001; Glaser *et al.*, 1995).

The hydroxyl O atoms (O1 and O2) of the phenol group act as donor atoms, forming intermolecular hydrogen bonds with atoms N11 and N22 of the triazole ring (Table 2). As shown in Fig. 2, these intermolecular O—H$\cdots$N hydrogen bonds link the molecules into two independent one-dimensional chains extending along the **c** direction.

Experimental

3-(1*H*-1,2,4-Triazol-4-yl)phenol was prepared by reacting diformylhydrazine (0.6 mmol, 0.053 g) and *m*-aminophenol (0.6 mmol, 0.065 g) in a Teflon-lined stainless steel autoclave in a furnace at 443 K for 3 d. The reaction vessel was then cooled to 293 K. The product was isolated and washed with hot water and hot ethanol and orange crystals suitable for X-ray diffraction studies were obtained. The crystals are air-stable. Yield based on *m*-aminophenol: 0.079 g, 82%. Elemental analysis (%) for $C_8H_7N_3O$, found (calculated): C 59.61 (59.62), H 4.29 (4.38), N 26.18 (25.90). IR (cm^{-1}, KBr): 3136 (*w*), 3120 (*w*), 2954 (*w*), 2846 (*w*), 2743 (*w*), 1613 (*s*), 1533 (*vs*), 1494 (*s*), 1388 (*w*), 1381 (*m*), 1293 (*s*), 1204 (*s*), 1093 (*m*). The electronic emission spectrum of the solid has a high-energy emission at *ca* 422 nm which can be assigned to the π–π^* transition and has a small red-shift as compared with that of *m*-aminophenol (λ_{em} = 415 nm). In the UV–Vis spectrum, two intense absorption peaks at *ca* 254 and 294 nm can be assigned to the π–π^* transition of the phenol ring and *the* n–π^* transition of the triazole ring, respectively.

Crystal data

$C_8H_7N_3O$
$M_r = 161.17$
Orthorhombic, *Pbca*
$a = 10.099$ (5) Å
$b = 16.315$ (7) Å
$c = 18.593$ (8) Å
$V = 3064$ (2) Å^3
$Z = 16$
$D_x = 1.398$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 6856 reflections
$\theta = 1.1$–$28.3°$
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Prism, yellow
0.50 × 0.30 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*SPHERE* in *CrystalClear*; Rigaku, 2002)
$T_{min} = 0.924$, $T_{max} = 0.988$
18 275 measured reflections

2685 independent reflections
2523 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.0°$
$h = -11 \rightarrow 12$
$k = -18 \rightarrow 19$
$l = -22 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.119$
$S = 1.27$
2685 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.89P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N11—C11	1.300 (3)	N21—C21	1.298 (3)
N11—N12	1.377 (3)	N21—N22	1.378 (3)
N12—C12	1.299 (3)	N22—C22	1.297 (3)
N13—C12	1.347 (2)	N23—C21	1.349 (3)
N13—C11	1.349 (2)	N23—C22	1.353 (3)
N13—C13	1.440 (2)	N23—C23	1.436 (2)
C12—N13—C11	103.92 (16)	C21—N23—C22	102.96 (17)
C12—N13—C13	128.55 (16)	C21—N23—C23	128.98 (16)
C11—N13—C13	127.51 (16)	C22—N23—C23	127.99 (18)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O2—H2O$\cdots$N22^{i}	0.89 (3)	1.91 (3)	2.779 (2)	169 (3)
O1—H1O$\cdots$N11^{ii}	0.95 (3)	1.76 (3)	2.707 (2)	174 (3)

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

H atoms bonded to C atoms were placed in calculated positions, with C—H distances of 0.93 Å, and included in the refinement in a riding-model approximation, with $U_{iso} = 1.2U_{eq}$ of the carrier atom. Hydroxyl H atoms were located in a difference map and refined with isotropic displacement parameters

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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