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2-[(*E*)-(2-Phenyl-2*H*-1,2,3-triazol-4-yl)-methyleneamino]ethanol

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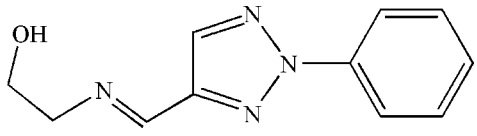
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.009 Å; R factor = 0.057; wR factor = 0.135; data-to-parameter ratio = 8.2.

In the title Schiff base compound, $C_{11}H_{12}N_4O$, the molecule adopts a *trans* configuration about the central C=N bond. The dihedral angle between the phenyl ring and the triazole ring is 14.3 (3)°. In the crystal structure, molecules are linked into a one-dimensional supramolecular chain by intermolecular O—H···N hydrogen bonding between the hydroxyl group and the imino N atom.

Related literature

For related literature on Schiff bases, see: Ali *et al.* (2002); Borisova *et al.* (2007); Maheswari *et al.* (2006). For the crystal structures of similar Schiff bases, see: Nate *et al.* (1987); Yogavel *et al.* (2003). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_{12}N_4O$
M_r = 216.25
Orthorhombic, $Pca2_1$
a = 13.124 (5) Å
b = 12.770 (5) Å
c = 6.658 (3) Å
V = 1115.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.12 × 0.07 × 0.03 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.989, T_{max} = 0.993
5534 measured reflections
1196 independent reflections
596 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.135
S = 1.01
1196 reflections
146 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N4^{i}	0.82	2.02	2.835 (6)	173

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2313).

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2-[(*E*)-(2-Phenyl-2*H*-1,2,3-triazol-4-yl)methyleneamino]ethanol

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S1. Comment

Schiff bases play an important role in coordination chemistry and have demonstrated significant biological activity (Ali *et al.*, 2002; Borisova *et al.*, 2007; Maheswari *et al.*, 2006). The title compound, derived from 2-phenyl-2*H*-1,2,3-triazole-4-carbaldehyde and 2-aminoethanol, is a potential N_3O tetradentate Schiff base ligand. Its crystal structure is described here.

The title molecule (Fig. 1) adopts a *trans* configuration about the central C═N bond. The dihedral angle between the phenyl ring and the triazole ring is 14.3 (3)°. Atoms C9 and N4 are nearly coplanar with the triazole ring; the maximum deviation from the mean plane through these seven atoms is 0.066 (7) Å for C9. The torsion angles C8—C7—C9—N4 and N3—C7—C9—N4 are 8.4 (11) and -173.2 (6)°, respectively. The bond lengths (Allen *et al.*, 1987) and angles of the molecule are within normal ranges. The N4═C9 [1.255 (5) Å] and N4—C10 [1.461 (5) Å] bond distances are comparable to those found in similar Schiff base compounds, such as 2-(2-(2-(4-phenylpiperazinyl)ethoxy)benzylideneamino)ethanol (Nate *et al.*, 1987) and 1,4-bis(2-hydroxy-3-(*N*-(2-hydroxyethyl)imino)-5-methylbenzyl)piperazine (Yogavel *et al.*, 2003). In the crystal structure, O1—H1···N4 intermolecular hydrogen bonds (Table 1 and Fig. 2), formed between the hydroxyl group and the imino N, link the molecules into a one-dimension supramolecular chain.

S2. Experimental

2-Phenyl-2*H*-1,2,3-triazole-4-carbaldehyde (0.17 g, 1 mmol) and 2-aminoethanol (0.06 g, 1 mmol) were refluxed for 30 min in a methanol solution (15 ml). The reaction mixture was cooled to room temprature and filtered. After allowing the filtrate to stand in air for 3 d, pale yellow plate crystals (yield 76%; mp 346–347 K) were obtained.

S3. Refinement

H atoms were placed at calculated positions and refined in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2 H atoms, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene H atoms, and O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(C) for the hydroxyl H atom. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

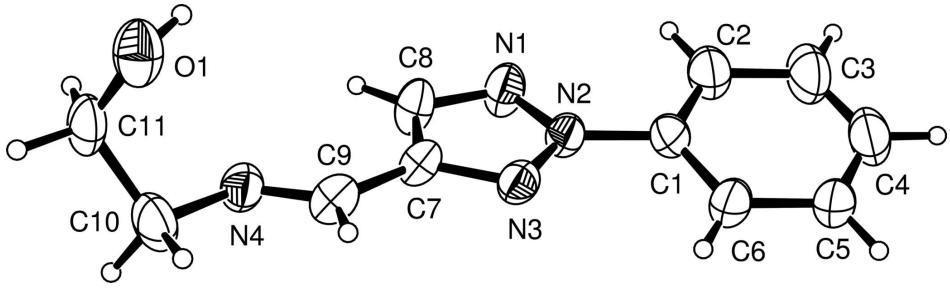

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

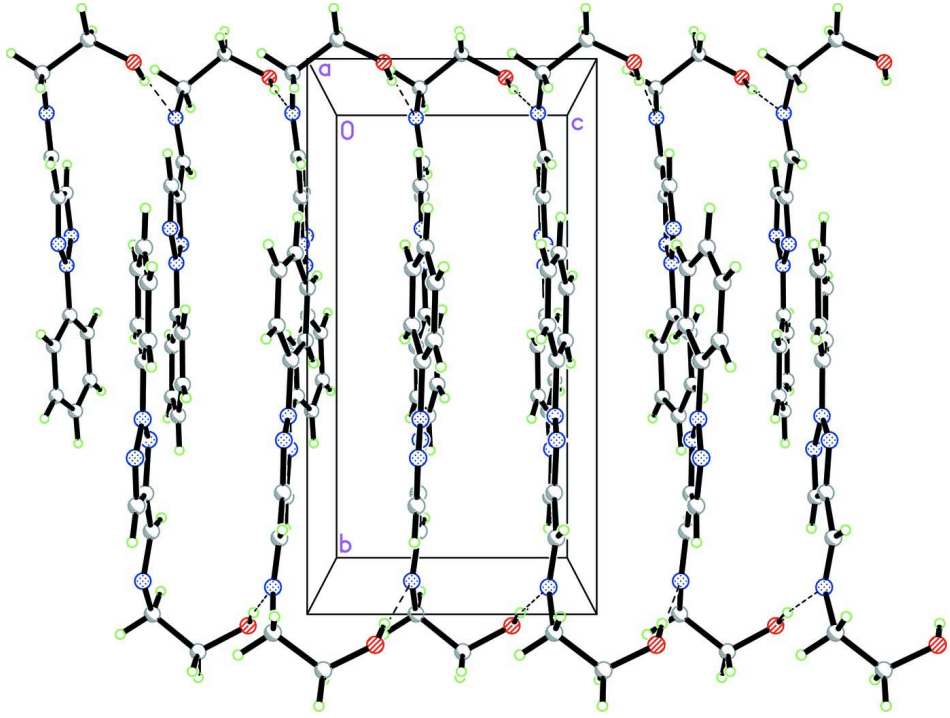

Figure 2

The packing of the title compound, viewed down the *a* axis. The intermolecular hydrogen bonds are shown as dashed lines.

2-[(*E*)-(2-Phenyl-2*H*-1,2,3-triazol-4-yl)methyleneamino]ethanol

Crystal data

$C_{11}H_{12}N_4O$
$M_r = 216.25$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 13.124\ (5)$ Å
$b = 12.770\ (5)$ Å
$c = 6.658\ (3)$ Å
$V = 1115.8\ (8)$ Å^3
$Z = 4$
$F(000) = 456$
$D_x = 1.287$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 320 reflections
$\theta = 2.2–18.5°$
$\mu = 0.09$ mm^{-1}
$T = 295$ K
Plate, pale yellow
0.12 × 0.07 × 0.03 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.989, T_{max} = 0.993
5534 measured reflections
1196 independent reflections
596 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 26.0°, θ_{min} = 1.6°
h = −16→16
k = −13→15
l = −7→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.135
S = 1.01
1196 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 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 $F^2 > \sigma(F^2)$ 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}
N1	0.0897 (3)	0.2763 (3)	0.8805 (10)	0.0761 (13)
N2	0.1661 (3)	0.3447 (3)	0.8868 (7)	0.0596 (11)
N3	0.2589 (3)	0.3020 (3)	0.8840 (7)	0.0578 (10)
N4	0.3009 (3)	0.0258 (3)	0.8507 (8)	0.0687 (13)
O1	0.3829 (3)	−0.0715 (3)	1.2273 (8)	0.0842 (13)
H1	0.3311	−0.0391	1.2570	0.126*
C1	0.1492 (4)	0.4541 (4)	0.8940 (10)	0.0680 (14)
C2	0.0539 (5)	0.4918 (4)	0.9368 (10)	0.084 (2)
H2	0.0006	0.4456	0.9619	0.101*
C3	0.0372 (6)	0.5982 (5)	0.9427 (11)	0.103 (3)
H3	−0.0274	0.6241	0.9718	0.123*
C4	0.1147 (7)	0.6647 (5)	0.9060 (11)	0.113 (3)
H4	0.1035	0.7365	0.9139	0.136*
C5	0.2086 (6)	0.6287 (4)	0.8579 (11)	0.107 (2)
H5	0.2605	0.6758	0.8274	0.128*
C6	0.2278 (5)	0.5209 (4)	0.8539 (9)	0.0877 (19)

H6	0.2925	0.4954	0.8247	0.105*
C7	0.2401 (3)	0.2000 (3)	0.8766 (9)	0.0602 (13)
C8	0.1364 (3)	0.1845 (4)	0.8733 (11)	0.0720 (15)
H8	0.1041	0.1197	0.8669	0.086*
C9	0.3212 (4)	0.1209 (4)	0.8771 (10)	0.0673 (14)
H9	0.3884	0.1414	0.8972	0.081*
C10	0.3852 (3)	−0.0487 (4)	0.8635 (14)	0.0854 (19)
H10A	0.4489	−0.0112	0.8791	0.103*
H10B	0.3888	−0.0894	0.7408	0.103*
C11	0.3691 (4)	−0.1209 (4)	1.0410 (13)	0.077 (2)
H11A	0.3006	−0.1491	1.0349	0.093*
H11B	0.4163	−0.1791	1.0308	0.093*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.066 (2)	0.051 (2)	0.111 (4)	−0.004 (2)	0.003 (4)	0.007 (4)
N2	0.076 (3)	0.046 (2)	0.057 (3)	−0.001 (2)	0.002 (3)	0.005 (3)
N3	0.071 (2)	0.052 (2)	0.051 (3)	−0.0108 (19)	−0.002 (3)	0.001 (3)
N4	0.063 (2)	0.054 (2)	0.089 (4)	0.005 (2)	0.012 (3)	0.009 (3)
O1	0.070 (3)	0.066 (3)	0.117 (4)	0.0067 (19)	−0.014 (2)	−0.001 (3)
C1	0.100 (4)	0.052 (3)	0.053 (4)	−0.004 (3)	0.008 (4)	−0.006 (4)
C2	0.105 (4)	0.062 (4)	0.086 (6)	0.009 (3)	0.001 (4)	−0.005 (3)
C3	0.156 (7)	0.061 (4)	0.092 (6)	0.023 (4)	−0.005 (5)	0.002 (4)
C4	0.207 (9)	0.055 (4)	0.077 (6)	0.013 (5)	0.013 (7)	−0.010 (4)
C5	0.181 (8)	0.057 (4)	0.083 (6)	−0.028 (4)	0.043 (6)	−0.011 (4)
C6	0.132 (5)	0.056 (3)	0.075 (5)	−0.023 (3)	0.020 (5)	−0.004 (4)
C7	0.064 (3)	0.050 (3)	0.066 (4)	−0.008 (2)	−0.001 (4)	0.013 (3)
C8	0.068 (3)	0.047 (3)	0.101 (5)	0.000 (2)	−0.012 (5)	0.012 (4)
C9	0.063 (3)	0.066 (3)	0.073 (4)	−0.007 (2)	−0.004 (4)	0.014 (5)
C10	0.069 (3)	0.064 (3)	0.124 (6)	0.018 (3)	0.017 (5)	−0.011 (5)
C11	0.055 (3)	0.045 (3)	0.132 (7)	0.012 (3)	0.010 (4)	0.007 (5)

Geometric parameters (Å, º)

N1—C8	1.324 (5)	C4—C5	1.354 (8)
N1—N2	1.330 (5)	C4—H4	0.9300
N2—N3	1.336 (5)	C5—C6	1.400 (7)
N2—C1	1.415 (6)	C5—H5	0.9300
N3—C7	1.327 (5)	C6—H6	0.9300
N4—C9	1.255 (5)	C7—C8	1.376 (6)
N4—C10	1.461 (5)	C7—C9	1.468 (6)
O1—C11	1.403 (8)	C8—H8	0.9300
O1—H1	0.8200	C9—H9	0.9300
C1—C6	1.365 (7)	C10—C11	1.514 (9)
C1—C2	1.371 (7)	C10—H10A	0.9700
C2—C3	1.377 (7)	C10—H10B	0.9700
C2—H2	0.9300	C11—H11A	0.9700

C3—C4	1.347 (9)	C11—H11B	0.9700
C3—H3	0.9300		
C8—N1—N2	103.5 (4)	C1—C6—H6	120.8
N1—N2—N3	114.8 (3)	C5—C6—H6	120.8
N1—N2—C1	122.1 (4)	N3—C7—C8	109.0 (4)
N3—N2—C1	123.1 (4)	N3—C7—C9	122.7 (4)
C7—N3—N2	103.4 (3)	C8—C7—C9	128.3 (4)
C9—N4—C10	117.4 (4)	N1—C8—C7	109.3 (4)
C11—O1—H1	109.5	N1—C8—H8	125.4
C6—C1—C2	120.8 (5)	C7—C8—H8	125.4
C6—C1—N2	119.5 (5)	N4—C9—C7	120.7 (4)
C2—C1—N2	119.7 (5)	N4—C9—H9	119.6
C1—C2—C3	119.8 (6)	C7—C9—H9	119.6
C1—C2—H2	120.1	N4—C10—C11	109.7 (5)
C3—C2—H2	120.1	N4—C10—H10A	109.7
C4—C3—C2	119.8 (7)	C11—C10—H10A	109.7
C4—C3—H3	120.1	N4—C10—H10B	109.7
C2—C3—H3	120.1	C11—C10—H10B	109.7
C3—C4—C5	121.1 (6)	H10A—C10—H10B	108.2
C3—C4—H4	119.4	O1—C11—C10	113.5 (5)
C5—C4—H4	119.4	O1—C11—H11A	108.9
C4—C5—C6	120.1 (6)	C10—C11—H11A	108.9
C4—C5—H5	119.9	O1—C11—H11B	108.9
C6—C5—H5	119.9	C10—C11—H11B	108.9
C1—C6—C5	118.3 (6)	H11A—C11—H11B	107.7
C8—N1—N2—N3	0.0 (8)	C2—C1—C6—C5	0.1 (10)
C8—N1—N2—C1	179.4 (6)	N2—C1—C6—C5	178.7 (6)
N1—N2—N3—C7	−0.3 (7)	C4—C5—C6—C1	1.8 (11)
C1—N2—N3—C7	−179.8 (5)	N2—N3—C7—C8	0.5 (7)
N1—N2—C1—C6	−165.0 (6)	N2—N3—C7—C9	−178.2 (5)
N3—N2—C1—C6	14.4 (9)	N2—N1—C8—C7	0.4 (8)
N1—N2—C1—C2	13.6 (10)	N3—C7—C8—N1	−0.6 (8)
N3—N2—C1—C2	−166.9 (6)	C9—C7—C8—N1	178.0 (6)
C6—C1—C2—C3	−1.0 (11)	C10—N4—C9—C7	−176.9 (6)
N2—C1—C2—C3	−179.6 (6)	N3—C7—C9—N4	−173.2 (6)
C1—C2—C3—C4	0.1 (11)	C8—C7—C9—N4	8.4 (11)
C2—C3—C4—C5	1.8 (12)	C9—N4—C10—C11	115.1 (7)
C3—C4—C5—C6	−2.8 (12)	N4—C10—C11—O1	−71.2 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N4^{i}	0.82	2.02	2.835 (6)	173

Symmetry code: (i) −*x*+1/2, *y*, *z*+1/2.