Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-2-Methoxy-6-[(5-methylisoxazol-3-yl)-iminomethyl]phenol

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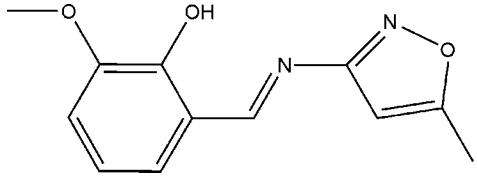
Received 9 December 2007; accepted 18 January 2008

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.122; data-to-parameter ratio = 6.9.

In the title molecule, $C_{12}H_{12}N_2O_3$, the benzene and isoxazole rings form a dihedral angle of 5.9 (6)°. The hydroxy group is involved in an intramolecular O—H···N hydrogen bond [O···N = 2.616 (5) Å], resulting in approximate planarity of the molecular skeleton. In the crystal structure, molecules related by translation along the c axis are stacked into columns, the shortest intermolecular C···C distance being 3.298 (6) Å.

Related literature

For related crystal structures, see Li *et al.* (2007). For general background, see Garnovskii *et al.* (1993).



Experimental

Crystal data

$C_{12}H_{12}N_2O_3$
M_r = 232.24
Orthorhombic, $Pna2_1$
a = 22.254 (5) Å
b = 10.178 (5) Å
c = 4.836 (2) Å
V = 1095.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 273 (2) K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.988, T_{max} = 0.992
3720 measured reflections
1079 independent reflections
651 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.122
S = 1.02
1079 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.89	2.616 (5)	147

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); 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*.

The authors thank the Postgraduate Foundation of Taishan University for financial support (grant No. Y06-2-12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2374).

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supporting information

Acta Cryst. (2008). E**64**, o499 [doi:10.1107/S1600536808001888]

(*E*)-2-Methoxy-6-[(5-methylisoxazol-3-yl)iminomethyl]phenol

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S1. Comment

Recently, a number of Schiff-bases have been investigated in terms of their crystallography and coordination chemistry (Garnovskii *et al.*, 1993). In continuation of our studies of Schiff-bases, we report here the synthesis and crystal structure of the title compound, (I).

In (I) (Fig. 1), the geometric parameters are in good agreement with those found in 2,4-di-*tert*-butyl-6-(4-chlorophenyl-iminomethyl)phenol (Li *et al.*, 2007). The benzene and the isoxazole rings make a dihedral angle of 5.9 (6)°. The hydroxy group is involved in intramolecular O—H···N hydrogen bond (Table 2). In the crystal, the molecules related by translation along *c* axis are stacked into columns with the shortest intermolecular C···C distance of 3.298 (6) Å (Table 1), suggesting an existence of $\pi\cdots\pi$ interactions.

S2. Experimental

The title compound was synthesized by the reaction of 2-hydroxy-3-methoxybenzaldehyde (0.152 g, 1 mmol) and 5-methylisoxazol-3-amine (0.098 g, 1 mmol) in ethanol solution and stirred under reflux conditions (353 K) for 6 h. When cooled to room temperature the solution was filtered and after a week orange crystals suitable for X-ray diffraction study were obtained. Yield, 0.186 g, 80%. m.p. 365–367 K.

Analysis found: C 61.98, H 5.25, N 12.04%; $C_{12}H_{12}N_2O_3$ requires: C 62.02, H 5.21, N 12.06%.

S3. Refinement

The H atoms were geometrically positioned (C—H 0.93–0.96 Å, O—H = 0.82 Å) and refined in a riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C-aromatic) and U_{iso}(H) = 1.5U_{eq}(*C*-methyl and O). Due to the absence of any significant anomalous scatterers in the molecule, the 758 Friedel pairs were merged before the final refinement.

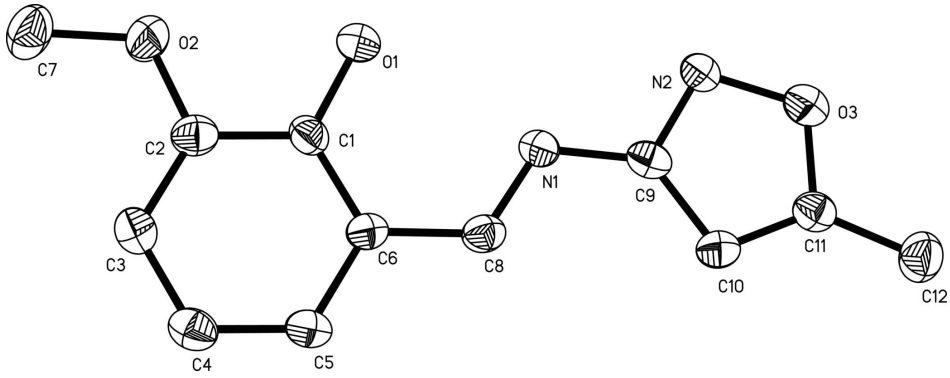

Figure 1

The molecular structure showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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Crystal data

$C_{12}H_{12}N_2O_3$
$M_r = 232.24$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 22.254$ (5) Å
$b = 10.178$ (5) Å
$c = 4.836$ (2) Å
$V = 1095.4$ (8) Å^3
$Z = 4$
$F(000) = 488$
$D_x = 1.408$ Mg m^{-3}
$D_m = 1.408$ Mg m^{-3}
D_m measured by not measured
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 401 reflections
$\theta = 2.7$–$18.4°$
$\mu = 0.10$ mm^{-1}
$T = 273$ K
Block, orange
0.12 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.988$, $T_{max} = 0.992$
3720 measured reflections
1079 independent reflections
651 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.8°$
$h = -26 \rightarrow 12$
$k = -11 \rightarrow 10$
$l = -5 \rightarrow 5$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.122$
$S = 1.02$
1079 reflections
156 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.009 (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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.38927 (16)	0.1624 (3)	0.1475 (8)	0.0589 (12)
H1	0.3605	0.1711	0.0433	0.088*

O2	0.47481 (17)	0.1609 (3)	0.5178 (8)	0.0642 (12)
O3	0.19927 (17)	0.2331 (3)	−0.6386 (9)	0.0630 (12)
N1	0.30586 (18)	0.2894 (4)	−0.1253 (10)	0.0435 (11)
N2	0.2451 (2)	0.1937 (4)	−0.4528 (11)	0.0600 (14)
C1	0.3990 (2)	0.2760 (5)	0.2836 (10)	0.0439 (14)
C2	0.4440 (2)	0.2775 (5)	0.4844 (12)	0.0493 (15)
C3	0.4554 (2)	0.3904 (5)	0.6332 (11)	0.0507 (14)
H3	0.4856	0.3913	0.7660	0.061*
C4	0.4214 (2)	0.5035 (5)	0.5842 (12)	0.0521 (15)
H4	0.4286	0.5792	0.6867	0.062*
C5	0.3773 (2)	0.5031 (5)	0.3843 (12)	0.0488 (13)
H5	0.3551	0.5790	0.3520	0.059*
C6	0.3655 (2)	0.3901 (5)	0.2295 (10)	0.0408 (13)
C7	0.5192 (3)	0.1552 (6)	0.7308 (13)	0.0709 (19)
H7A	0.5505	0.2174	0.6920	0.106*
H7B	0.5359	0.0683	0.7384	0.106*
H7C	0.5009	0.1760	0.9054	0.106*
C8	0.3197 (2)	0.3922 (5)	0.0215 (11)	0.0448 (13)
H8	0.2990	0.4702	−0.0098	0.054*
C9	0.2608 (2)	0.3021 (5)	−0.3245 (11)	0.0457 (14)
C10	0.2266 (2)	0.4109 (5)	−0.4155 (12)	0.0512 (15)
H10	0.2295	0.4971	−0.3536	0.061*
C11	0.1892 (2)	0.3643 (5)	−0.6087 (11)	0.0464 (14)
C12	0.1426 (2)	0.4195 (6)	−0.7923 (12)	0.0658 (18)
H12A	0.1372	0.3628	−0.9489	0.099*
H12B	0.1548	0.5050	−0.8544	0.099*
H12C	0.1054	0.4266	−0.6928	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.069 (3)	0.040 (2)	0.068 (3)	0.0036 (19)	−0.016 (2)	−0.009 (2)
O2	0.068 (3)	0.056 (2)	0.069 (3)	0.016 (2)	−0.019 (2)	−0.004 (2)
O3	0.070 (3)	0.049 (2)	0.070 (3)	−0.006 (2)	−0.013 (2)	−0.007 (2)
N1	0.045 (3)	0.036 (2)	0.049 (2)	−0.002 (2)	−0.002 (2)	−0.003 (2)
N2	0.068 (3)	0.041 (3)	0.071 (3)	−0.009 (2)	−0.027 (3)	0.002 (3)
C1	0.046 (3)	0.041 (3)	0.045 (3)	−0.009 (3)	−0.004 (3)	0.000 (3)
C2	0.049 (4)	0.044 (3)	0.056 (4)	0.003 (3)	0.007 (3)	−0.001 (3)
C3	0.048 (3)	0.055 (3)	0.049 (3)	−0.003 (3)	−0.002 (3)	−0.005 (3)
C4	0.060 (4)	0.044 (3)	0.052 (3)	−0.009 (3)	0.006 (3)	−0.002 (3)
C5	0.056 (3)	0.036 (3)	0.055 (3)	−0.001 (3)	0.000 (4)	−0.004 (3)
C6	0.041 (3)	0.034 (3)	0.047 (3)	0.002 (3)	0.003 (3)	0.001 (2)
C7	0.069 (4)	0.078 (4)	0.065 (4)	0.027 (3)	−0.011 (4)	−0.002 (4)
C8	0.042 (3)	0.038 (3)	0.055 (3)	0.004 (3)	0.004 (3)	0.000 (3)
C9	0.050 (4)	0.038 (3)	0.049 (3)	−0.007 (3)	0.008 (3)	−0.003 (3)
C10	0.056 (4)	0.039 (3)	0.059 (4)	0.007 (3)	−0.003 (3)	−0.007 (3)
C11	0.047 (4)	0.045 (3)	0.048 (3)	−0.001 (3)	0.007 (3)	−0.006 (3)
C12	0.064 (4)	0.073 (4)	0.061 (4)	0.008 (3)	−0.011 (4)	−0.005 (4)

Geometric parameters (Å, º)

O1—C1	1.348 (5)	C4—H4	0.9300
O1—H1	0.8200	C5—C6	1.397 (7)
O2—C2	1.379 (6)	C5—H5	0.9300
O2—C7	1.428 (6)	C6—C8	1.433 (7)
O3—C11	1.362 (6)	C7—H7A	0.9600
O3—N2	1.417 (6)	C7—H7B	0.9600
N1—C8	1.301 (6)	C7—H7C	0.9600
N1—C9	1.397 (7)	C8—H8	0.9300
N2—C9	1.313 (5)	C9—C10	1.413 (6)
C1—C2	1.395 (7)	C10—C11	1.338 (7)
C1—C6	1.405 (7)	C10—H10	0.9300
C2—C3	1.379 (7)	C11—C12	1.477 (7)
C3—C4	1.397 (7)	C12—H12A	0.9600
C3—H3	0.9300	C12—H12B	0.9600
C4—C5	1.377 (7)	C12—H12C	0.9600
C4···C8^{i}	3.298 (6)	C6···C9^{i}	3.299 (6)
C1—O1—H1	109.5	O2—C7—H7B	109.5
C2—O2—C7	117.5 (4)	H7A—C7—H7B	109.5
C11—O3—N2	109.2 (4)	O2—C7—H7C	109.5
C8—N1—C9	118.2 (4)	H7A—C7—H7C	109.5
C9—N2—O3	104.7 (4)	H7B—C7—H7C	109.5
O1—C1—C2	117.7 (5)	N1—C8—C6	122.6 (5)
O1—C1—C6	122.2 (5)	N1—C8—H8	118.7
C2—C1—C6	120.1 (5)	C6—C8—H8	118.7
O2—C2—C3	124.4 (5)	N2—C9—N1	116.0 (5)
O2—C2—C1	115.4 (5)	N2—C9—C10	111.6 (5)
C3—C2—C1	120.2 (5)	N1—C9—C10	132.3 (5)
C2—C3—C4	119.9 (5)	C11—C10—C9	106.0 (5)
C2—C3—H3	120.0	C11—C10—H10	127.0
C4—C3—H3	120.0	C9—C10—H10	127.0
C5—C4—C3	120.1 (5)	C10—C11—O3	108.6 (5)
C5—C4—H4	119.9	C10—C11—C12	136.3 (5)
C3—C4—H4	119.9	O3—C11—C12	115.1 (5)
C4—C5—C6	120.8 (5)	C11—C12—H12A	109.5
C4—C5—H5	119.6	C11—C12—H12B	109.5
C6—C5—H5	119.6	H12A—C12—H12B	109.5
C5—C6—C1	118.8 (5)	C11—C12—H12C	109.5
C5—C6—C8	119.8 (5)	H12A—C12—H12C	109.5
C1—C6—C8	121.4 (5)	H12B—C12—H12C	109.5
O2—C7—H7A	109.5		
C11—O3—N2—C9	−0.8 (5)	O1—C1—C6—C8	−1.2 (7)
C7—O2—C2—C3	3.5 (8)	C2—C1—C6—C8	179.0 (4)
C7—O2—C2—C1	−176.8 (4)	C9—N1—C8—C6	−179.5 (4)

O1—C1—C2—O2	1.2 (7)	C5—C6—C8—N1	−178.6 (5)
C6—C1—C2—O2	−179.0 (5)	C1—C6—C8—N1	1.0 (7)
O1—C1—C2—C3	−179.0 (5)	O3—N2—C9—N1	179.6 (4)
C6—C1—C2—C3	0.8 (7)	O3—N2—C9—C10	0.8 (6)
O2—C2—C3—C4	−179.8 (5)	C8—N1—C9—N2	−175.0 (5)
C1—C2—C3—C4	0.5 (8)	C8—N1—C9—C10	3.5 (8)
C2—C3—C4—C5	−1.1 (8)	N2—C9—C10—C11	−0.5 (6)
C3—C4—C5—C6	0.5 (8)	N1—C9—C10—C11	−179.0 (5)
C4—C5—C6—C1	0.8 (7)	C9—C10—C11—O3	−0.1 (5)
C4—C5—C6—C8	−179.6 (4)	C9—C10—C11—C12	−178.7 (6)
O1—C1—C6—C5	178.4 (5)	N2—O3—C11—C10	0.6 (5)
C2—C1—C6—C5	−1.4 (7)	N2—O3—C11—C12	179.5 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.89	2.616 (5)	147