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2-(2-Methoxyphenyl)-4,4-dimethyl-4,5-dihydro-1,3-oxazole

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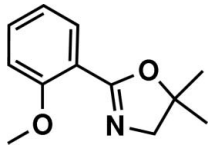
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.001 Å; R factor = 0.048; wR factor = 0.163; data-to-parameter ratio = 26.9.

In the title molecule, $C_{12}H_{15}NO_2$, the oxazole ring adopts an envelope conformation. Overall, the molecule is approximately planar, the dihedral angle between the mean plane through all but the methylene C atom of the five-membered ring and the aromatic ring being 8.6 (1)°. A weak C—H···O interaction contributes to the stabilization of the crystal structure.

Related literature

For related crystal structures, see: Swaleh & Ziemer (2001); Rybakov *et al.* (2006).



Experimental

Crystal data

$C_{12}H_{15}NO_2$
M_r = 205.25
Monoclinic, $P2_1/n$
a = 8.1495 (2) Å
b = 10.9369 (3) Å
c = 12.0864 (3) Å
β = 91.305 (3)°
V = 1076.99 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 200 (2) K
0.39 × 0.31 × 0.24 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.717, T_{max} = 1.000 (expected range = 0.702–0.980)
34412 measured reflections
3740 independent reflections
2596 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.163
S = 1.13
3740 reflections
139 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C26—H26···O1	0.93	2.35	2.7136 (12)	103

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2221).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Oxford Diffraction (2007). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171.32. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Rybakov, V. B., Alifanov, V. L. & Babaev, E. V. (2006). *Acta Cryst.* E**62**, o4746–o4747.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Swaleh, S. & Ziemer, B. (2001). *Acta Cryst.* E**57**, o35–o36.

supporting information

Acta Cryst. (2008). E**64**, o61 [https://doi.org/10.1107/S1600536807061685]

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S1. Comment

Swaleh and Ziemer (2001) reported the crystal structure of 2-[(2-phenyl-1,3-oxazol-4-yl)methyl]-2*H*-1,2,3-benzotriazole, wherein the phenyl and oxazole rings are essentially co-planar. Rybakov *et al.* (2006) reported the crystal structure of 5-(4-bromophenyl)-1,3-oxazol-2-amine, wherein the oxazole and the aromatic rings form a dihedral angle of 9.68 (7)°. In the title molecule, $C_{12}H_{15}NO_2$ (I), Fig. 1, the oxazole ring is in an envelope conformation. The dihedral angle between the mean plane through the O1/C2/N3/C5 atoms and that through the aromatic ring is 8.6 (1)°. A weak C—H···O interaction contributes to the stabilization of the crystal structure (Table 1).

S2. Experimental

To a solution of 2-methoxy benzyl chloride (15.8 g, 0.1 mol) in dichloromethane (50 ml), 2-amino-2-methyl-1-propanol (8.3 g, 0.11 mol) in dichloromethane (50 ml) was added at 298–303 K over 30 min. After stirring for 1 h, dichloromethane was distilled off under reduced pressure. The obtained product was recrystallized using ethyl acetate as the solvent to yield 10 g of (I) (86.5%).

S3. Refinement

The H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93–0.97 Å, and with U_{iso} = 1.2–1.5 times U_{eq}(C).

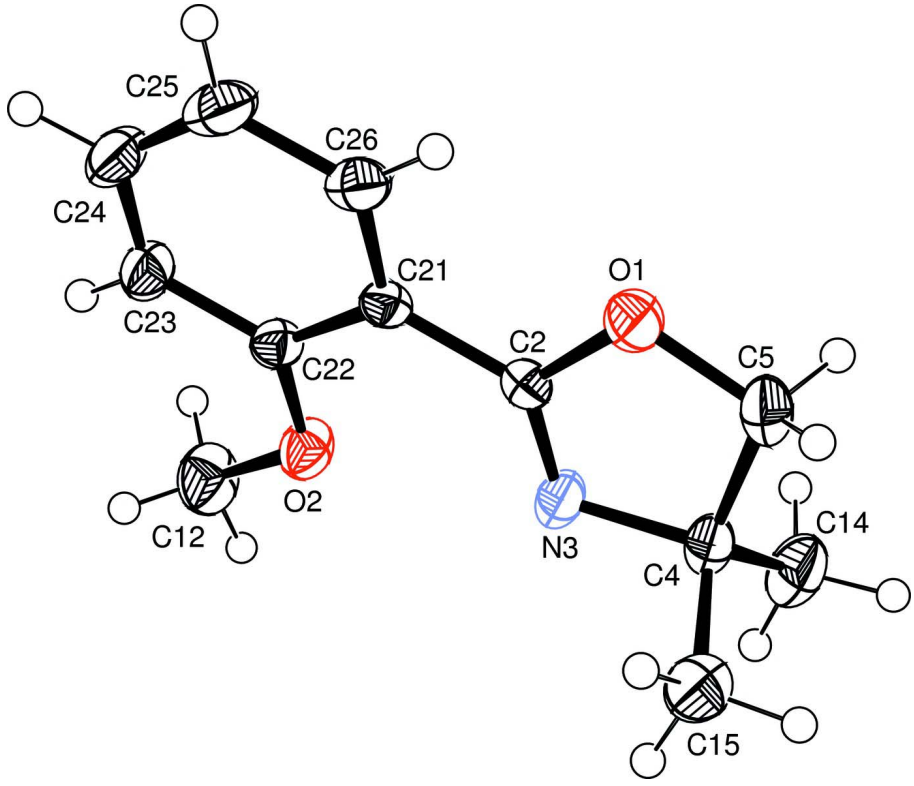

Figure 1

The molecular structure of (I) showing the atomic numbering and 50% probability displacement ellipsoids.

2-(2-Methoxyphenyl)-4,4-dimethyl-4,5-dihydro-1,3-oxazole

Crystal data

$C_{12}H_{15}NO_2$
$M_r = 205.25$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.1495$ (2) Å
$b = 10.9369$ (3) Å
$c = 12.0864$ (3) Å
$\beta = 91.305$ (3)°
$V = 1076.99$ (5) Å^3
$Z = 4$

$F(000) = 440$
$D_x = 1.266$ Mg m^{-3}
Melting point: 410(1) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14583 reflections
$\theta = 4.6$–$32.5°$
$\mu = 0.09$ mm^{-1}
$T = 200$ K
Prism, colourless
0.39 × 0.31 × 0.24 mm

Data collection

Oxford Diffraction Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.717$, $T_{max} = 1.000$

34412 measured reflections
3740 independent reflections
2596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 32.6°$, $\theta_{min} = 4.6°$
$h = -12 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.163$
$S = 1.13$
3740 reflections
139 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
$w = 1/[\sigma^2(F_o^2) + (0.099P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.61501 (9)	0.49026 (7)	0.33582 (5)	0.0357 (2)
O2	0.40996 (9)	0.22987 (6)	0.11696 (6)	0.0332 (2)
N3	0.65111 (10)	0.39575 (8)	0.17107 (7)	0.0325 (2)
C2	0.56870 (11)	0.40277 (7)	0.25852 (7)	0.0230 (2)
C4	0.78858 (13)	0.48460 (9)	0.18188 (8)	0.0310 (3)
C5	0.74394 (15)	0.55882 (10)	0.28508 (10)	0.0409 (3)
C12	0.33176 (17)	0.14486 (11)	0.04469 (10)	0.0445 (4)
C14	0.79827 (15)	0.56238 (11)	0.07847 (10)	0.0442 (4)
C15	0.94665 (14)	0.41267 (10)	0.20004 (11)	0.0428 (4)
C21	0.42972 (11)	0.32650 (8)	0.29281 (7)	0.0235 (2)
C22	0.35474 (11)	0.23841 (8)	0.22165 (7)	0.0254 (2)
C23	0.22969 (13)	0.16468 (9)	0.26164 (9)	0.0333 (3)
C24	0.18045 (13)	0.17635 (10)	0.37044 (10)	0.0389 (3)
C25	0.25034 (13)	0.26249 (11)	0.44046 (9)	0.0385 (3)
C26	0.37380 (12)	0.33708 (9)	0.40107 (8)	0.0300 (3)
H5A	0.83805	0.56661	0.33518	0.0491*
H5B	0.70600	0.63992	0.26448	0.0491*
H12A	0.38149	0.14833	−0.02649	0.0668*
H12B	0.21733	0.16474	0.03700	0.0668*
H12C	0.34348	0.06393	0.07459	0.0668*
H14A	0.82155	0.51117	0.01626	0.0662*
H14B	0.88401	0.62191	0.08799	0.0662*
H14C	0.69541	0.60335	0.06566	0.0662*
H15A	0.96128	0.35762	0.13920	0.0641*
H15B	0.94063	0.36683	0.26757	0.0641*
H15C	1.03780	0.46817	0.20484	0.0641*

H23	0.17905	0.10747	0.21531	0.0399*
H24	0.09887	0.12517	0.39659	0.0466*
H25	0.21528	0.27039	0.51280	0.0463*
H26	0.42061	0.39563	0.44781	0.0360*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0389 (4)	0.0352 (4)	0.0334 (4)	−0.0092 (3)	0.0072 (3)	−0.0128 (3)
O2	0.0348 (4)	0.0360 (4)	0.0288 (3)	−0.0099 (3)	0.0026 (3)	−0.0042 (3)
N3	0.0315 (4)	0.0313 (4)	0.0352 (4)	−0.0108 (3)	0.0101 (3)	−0.0042 (3)
C2	0.0250 (4)	0.0206 (4)	0.0234 (4)	0.0013 (3)	0.0010 (3)	−0.0022 (3)
C4	0.0303 (5)	0.0276 (5)	0.0352 (5)	−0.0080 (4)	0.0051 (4)	−0.0003 (4)
C5	0.0431 (6)	0.0303 (5)	0.0496 (7)	−0.0132 (5)	0.0087 (5)	−0.0089 (4)
C12	0.0492 (7)	0.0448 (6)	0.0394 (6)	−0.0134 (5)	−0.0026 (5)	−0.0095 (5)
C14	0.0402 (6)	0.0441 (6)	0.0483 (7)	−0.0097 (5)	0.0044 (5)	0.0124 (5)
C15	0.0354 (6)	0.0412 (6)	0.0519 (7)	−0.0010 (5)	0.0043 (5)	0.0036 (5)
C21	0.0220 (4)	0.0220 (4)	0.0266 (4)	0.0038 (3)	0.0031 (3)	0.0006 (3)
C22	0.0219 (4)	0.0258 (4)	0.0284 (4)	0.0018 (3)	0.0015 (3)	0.0011 (3)
C23	0.0246 (5)	0.0310 (5)	0.0443 (6)	−0.0041 (4)	0.0024 (4)	0.0026 (4)
C24	0.0267 (5)	0.0404 (6)	0.0500 (6)	−0.0010 (4)	0.0123 (4)	0.0112 (5)
C25	0.0335 (5)	0.0466 (6)	0.0361 (5)	0.0082 (5)	0.0135 (4)	0.0088 (4)
C26	0.0300 (5)	0.0328 (5)	0.0274 (4)	0.0066 (4)	0.0058 (4)	0.0037 (3)

Geometric parameters (Å, º)

O1—C2	1.3838 (11)	C5—H5A	0.9700
O1—C5	1.4393 (14)	C5—H5B	0.9700
O2—C12	1.4171 (14)	C12—H12A	0.9600
O2—C22	1.3558 (11)	C12—H12B	0.9600
N3—C2	1.2675 (12)	C12—H12C	0.9600
N3—C4	1.4865 (13)	C14—H14A	0.9600
C2—C21	1.4737 (12)	C14—H14B	0.9600
C4—C5	1.5387 (15)	C14—H14C	0.9600
C4—C14	1.5154 (16)	C15—H15A	0.9600
C4—C15	1.5211 (15)	C15—H15B	0.9600
C21—C22	1.4203 (12)	C15—H15C	0.9600
C21—C26	1.4001 (13)	C23—H23	0.9300
C22—C23	1.3946 (14)	C24—H24	0.9300
C23—C24	1.3895 (16)	C25—H25	0.9300
C24—C25	1.3807 (16)	C26—H26	0.9300
C25—C26	1.3879 (15)		
O1···C12^{i}	3.3873 (14)	H12B···H23	2.2700
O2···N3	2.7428 (11)	H12C···C23	2.7000
O1···H26^{ii}	2.9200	H12C···H23	2.2400
O1···H26	2.3500	H12C···C26^{xi}	3.0700
O1···H23^{iii}	2.7800	H14A···H15A	2.5000

O2···H5A^{iv}	2.7700	H14A···C24^{v}	2.9200
O2···H25^{v}	2.8100	H14B···H15C	2.5100
N3···O2	2.7428 (11)	H14B···C21^{x}	3.0500
N3···C25^{v}	3.3942 (14)	H14B···C26^{x}	3.0700
N3···H25^{v}	2.7000	H14C···H5B	2.4400
C12···O1^{vi}	3.3873 (14)	H14C···H24^{iii}	2.4600
C25···N3^{vii}	3.3942 (14)	H14C···C12^{viii}	3.0700
C2···H23^{iii}	3.0400	H15A···H14A	2.5000
C2···H15B	3.0600	H15B···C2	3.0600
C5···H25^{ii}	3.0900	H15B···C24^{xii}	3.1000
C12···H14C^{viii}	3.0700	H15B···H5A	2.4800
C12···H23	2.4700	H15B···H12A^{i}	2.5500
C21···H14B^{iv}	3.0500	H15C···H5A	2.5300
C23···H12B	2.7100	H15C···H14B	2.5100
C23···H12C	2.7000	H15C···C23^{x}	2.8900
C23···H15C^{iv}	2.8900	H23···C12	2.4700
C24···H15B^{ix}	3.1000	H23···H12B	2.2700
C24···H14A^{vii}	2.9200	H23···H12C	2.2400
C26···H12C^{iii}	3.0700	H23···O1^{xi}	2.7800
C26···H14B^{iv}	3.0700	H23···C2^{xi}	3.0400
H5A···H15B	2.4800	H24···H14C^{xi}	2.4600
H5A···H15C	2.5300	H25···C5^{ii}	3.0900
H5A···O2^{x}	2.7700	H25···O2^{vii}	2.8100
H5B···H14C	2.4400	H25···N3^{vii}	2.7000
H12A···H15B^{vi}	2.5500	H26···O1	2.3500
H12B···C23	2.7100	H26···O1^{ii}	2.9200

C2—O1—C5	105.25 (7)	H5A—C5—H5B	109.00
C12—O2—C22	117.79 (8)	O2—C12—H12A	109.00
C2—N3—C4	107.44 (8)	O2—C12—H12B	109.00
O1—C2—N3	117.61 (8)	O2—C12—H12C	109.00
O1—C2—C21	113.65 (7)	H12A—C12—H12B	109.00
N3—C2—C21	128.72 (8)	H12A—C12—H12C	109.00
N3—C4—C5	102.97 (8)	H12B—C12—H12C	109.00
N3—C4—C14	110.35 (8)	C4—C14—H14A	109.00
N3—C4—C15	107.98 (8)	C4—C14—H14B	109.00
C5—C4—C14	112.96 (9)	C4—C14—H14C	109.00
C5—C4—C15	111.78 (9)	H14A—C14—H14B	109.00
C14—C4—C15	110.46 (9)	H14A—C14—H14C	109.00
O1—C5—C4	105.01 (8)	H14B—C14—H14C	109.00
C2—C21—C22	122.44 (8)	C4—C15—H15A	109.00
C2—C21—C26	118.99 (8)	C4—C15—H15B	109.00
C22—C21—C26	118.51 (8)	C4—C15—H15C	109.00
O2—C22—C21	117.68 (8)	H15A—C15—H15B	109.00
O2—C22—C23	122.98 (8)	H15A—C15—H15C	109.00
C21—C22—C23	119.34 (8)	H15B—C15—H15C	109.00
C22—C23—C24	120.26 (9)	C22—C23—H23	120.00
C23—C24—C25	121.25 (10)	C24—C23—H23	120.00

C24—C25—C26	118.88 (10)	C23—C24—H24	119.00
C21—C26—C25	121.73 (9)	C25—C24—H24	119.00
O1—C5—H5A	111.00	C24—C25—H25	121.00
O1—C5—H5B	111.00	C26—C25—H25	121.00
C4—C5—H5A	111.00	C21—C26—H26	119.00
C4—C5—H5B	111.00	C25—C26—H26	119.00
C5—O1—C2—N3	5.16 (11)	N3—C4—C5—O1	12.97 (10)
C5—O1—C2—C21	−176.76 (8)	C14—C4—C5—O1	132.00 (9)
C2—O1—C5—C4	−11.14 (10)	C15—C4—C5—O1	−102.69 (10)
C12—O2—C22—C21	−177.98 (9)	C2—C21—C22—O2	−3.21 (13)
C12—O2—C22—C23	2.38 (13)	C2—C21—C22—C23	176.46 (8)
C4—N3—C2—O1	3.72 (11)	C26—C21—C22—O2	179.69 (8)
C4—N3—C2—C21	−174.03 (9)	C26—C21—C22—C23	−0.65 (13)
C2—N3—C4—C5	−10.28 (10)	C2—C21—C26—C25	−175.91 (9)
C2—N3—C4—C14	−131.11 (9)	C22—C21—C26—C25	1.29 (14)
C2—N3—C4—C15	108.08 (9)	O2—C22—C23—C24	178.86 (9)
O1—C2—C21—C22	174.63 (8)	C21—C22—C23—C24	−0.79 (14)
O1—C2—C21—C26	−8.28 (12)	C22—C23—C24—C25	1.65 (16)
N3—C2—C21—C22	−7.55 (15)	C23—C24—C25—C26	−1.01 (16)
N3—C2—C21—C26	169.54 (9)	C24—C25—C26—C21	−0.48 (16)

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1/2, y+1/2, -z+1/2$; (iv) $-x+3/2, y-1/2, -z+1/2$; (v) $x+1/2, -y+1/2, z-1/2$; (vi) $x-1/2, -y+1/2, z-1/2$; (vii) $x-1/2, -y+1/2, z+1/2$; (viii) $-x+1, -y+1, -z$; (ix) $x-1, y, z$; (x) $-x+3/2, y+1/2, -z+1/2$; (xi) $-x+1/2, y-1/2, -z+1/2$; (xii) $x+1, y, z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C26—H26···O1	0.93	2.35	2.7136 (12)	103