Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(5-Methyl-1,3,4-oxadiazol-2-yl)phenyl acetate

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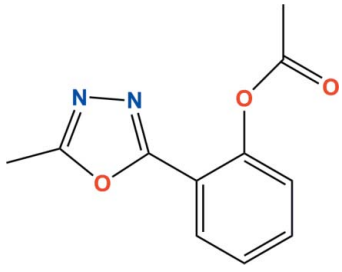
Received 21 January 2014; accepted 9 April 2014

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.136; data-to-parameter ratio = 12.9.

In the title compound, $C_{11}H_{10}N_2O_3$, which is a potential bioactive compound, the benzene and oxadiazole rings are approximately coplanar, with an inter-ring dihedral angle of 4.14 (2)°, while the ester plane is rotated out of the benzene plane [dihedral angle = 82.69 (9)°]. In the crystal, the molecules form layers down the a axis with weak π–π interactions between the oxadiazole and benzene rings [minimum ring centroid separation = 3.7706 (14) Å].

Related literature

For the bioactivity of 1,3,4-oxadiazole derivatives, see: Boström *et al.* (2012); Rajak *et al.* (2009); Polshettiwar & Varma (2008). For the properties of the 1,3,4-oxadiazole heterocycle, see: Bolton & Kim (2007); Liu *et al.* (2007); Kulkarni *et al.* (2004). For material chemistry applications, see: Hughes & Bryce (2005); Wang *et al.* (2011); Cristiano *et al.* (2006); Han (2013). For the synthesis, see: Gallardo *et al.* (2001). For related structures, see: Vencato *et al.* (1996); Gutov (2013).



Experimental

Crystal data

$C_{11}H_{10}N_2O_3$
M_r = 218.21
Monoclinic, $P2_1/n$
a = 6.6335 (6) Å
b = 16.925 (3) Å
c = 9.5078 (6) Å
β = 92.113 (6)°
V = 1066.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.50 × 0.36 × 0.16 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
1998 measured reflections
1885 independent reflections
1403 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.136
S = 1.11
1885 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *SET4* in *CAD-4 Software*; data reduction: *HELENA* (Spek, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors thank the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), the Fundação de Amparo à Pesquisa e Inovação do Estado de Santa Catarina (FAPESC), the Financiadora de Estudos e Projetos (FINEP) and the Instituto Nacional de Ciência e Tecnologia (INCT) - Catálise for financial assistance.

Supporting information for this paper is available from the IUCr electronic archives (Reference: ZS2285).

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supporting information

Acta Cryst. (2014). E**70**, o559 [doi:10.1107/S1600536814007946]

2-(5-Methyl-1,3,4-oxadiazol-2-yl)phenyl acetate

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S1. Comment

Molecules containing the heterocycle 1,3,4-oxadiazole exhibit a wide range of biological activities, such as anticancer, antidiabetic, anti-inflammatory, analgesic, antibacterial, anticonvulsant, anti-HIV, herbicidal, fungicidal, pesticidal and antihypertensive (Boström *et al.*, 2012; Rajak *et al.*, 2009). This five-membered ring has been studied as a potential pharmacophore in a variety of chemical structures, due to its favorable metabolic profile and its capability of forming H-bonding associations (Polshettiwar & Varma, 2008; Gutov, 2013). Furthermore, aromatic substituted 1,3,4-oxadiazoles have widely been used in electro-optical devices due to their good thermal and chemical stability, blue luminescence with high quantum yield and electron transporting capabilities (Hughes & Bryce, 2005; Han, 2013).

As part of our continuing interest in the synthesis and evaluation of bioactive molecules containing *N*-heterocycles, we now report the synthesis and structure of the title compound $C_{11}H_{10}N_2O_3$. In this structure (Fig. 1), the benzene and oxadiazole rings are approximately coplanar, with an inter-ring dihedral angle of 4.14 (2)°, while the ester plane defined by O1, O2, C13, C14 is rotated out of the benzene plane giving a dihedral angle of 82.69 (9)° which corresponds to a torsion angle C6—C7—O1—C13 of 83.26 (22)°. In the crystal the molecules form layers down the *a* axis with weak inter-layer π–π interactions between the oxadiazole and benzene rings [minimum ring centroid separation = 3.7706 (14) Å].

S2. Experimental

A mixture of 5-(2-hydroxyphenyl)tetrazole (Gallardo *et al.*, 2001) (2.0 g, 12.3 mmol) and acetic anhydride (6.3 g, 61.5 mmol) was heated under reflux for 2 h. The reaction mixture was poured into water/ice, the precipitate was filtered, washed with cold water and dried under vacuum to give the title compound as a white solid (1.88 g, 70%). Crystals suitable for X-ray diffraction were obtained from slow evaporation of the $CDCl_3$ solution. M.p.= 108 °C. ^{1}H NMR ($CDCl_3$) = 8.00 (dd, J = 7.8 and 1.6 Hz, 1H), 7.60 - 7.51 (m, 1H), 7.38 (t, J = 7.8 Hz, 1H), 7.23 (t, J = 7.8 Hz, 1H), 2.60 (s, 3H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$) = 169.88, 163.35, 162.12, 148.68, 132.67, 129.21, 126.60, 124.22, 117.65, 21.20, 11.08.

S3. Refinement

All non-H atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed at their idealized positions with distances of 0.93 Å for C—H_{Ar} and 0.96 Å for CH_3 groups and allowed to ride. Their U_{eq} were fixed at 1.2 and 1.5 times U_{iso} of the preceding atom for aromatic and methyl groups, respectively. H atoms of the methyl groups were treated as ideally disordered over two sites.

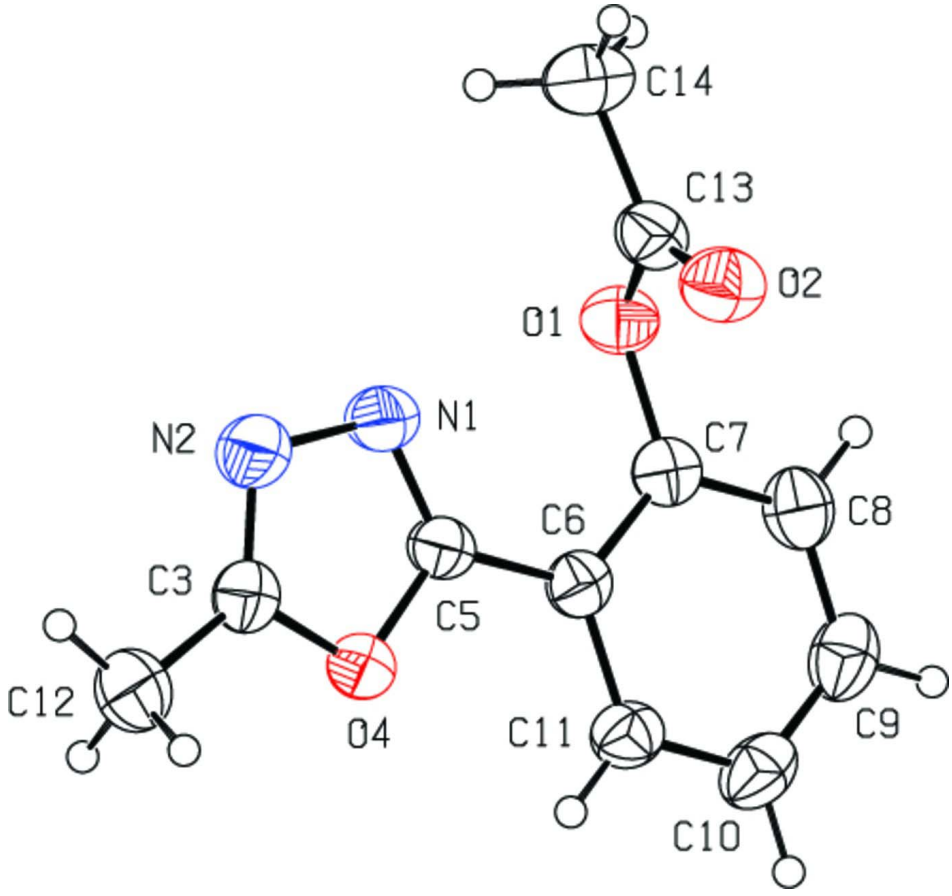

Figure 1

The molecular structure of the title compound with atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

2-(5-Methyl-1,3,4-oxadiazol-2-yl)phenyl acetate

Crystal data

$C_{11}H_{10}N_2O_3$
$M_r = 218.21$
Monoclinic, $P2_1/n$
$a = 6.6335$ (6) Å
$b = 16.925$ (3) Å
$c = 9.5078$ (6) Å
$\beta = 92.113$ (6)°
$V = 1066.7$ (2) Å^3
$Z = 4$
$F(000) = 456$
$D_x = 1.359$ Mg m^{-3}
Melting point: 381 K
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 6.5$–15.6°
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Block, colorless
0.50 × 0.36 × 0.16 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
ω–2θ scans
1998 measured reflections
1885 independent reflections
1403 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.1$°, $\theta_{min} = 2.4$°
$h = -7 \rightarrow 7$

$k = -20 \rightarrow 0$
$l = -11 \rightarrow 0$

3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.136$
$S = 1.11$
1885 reflections
146 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.1662P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.020 (4)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C3	0.7116 (3)	0.20207 (12)	0.5466 (2)	0.0529 (5)	
C5	0.7187 (3)	0.09558 (12)	0.42764 (19)	0.0449 (5)	
C6	0.7352 (3)	0.00994 (11)	0.4065 (2)	0.0438 (5)	
C7	0.7258 (3)	−0.02402 (12)	0.2733 (2)	0.0466 (5)	
C8	0.7460 (3)	−0.10475 (13)	0.2556 (2)	0.0572 (6)	
H8	0.7388	−0.1265	0.1658	0.069*	
C9	0.7766 (3)	−0.15261 (13)	0.3706 (3)	0.0613 (6)	
H9	0.7912	−0.2068	0.3587	0.074*	
C10	0.7858 (3)	−0.12053 (13)	0.5041 (3)	0.0602 (6)	
H10	0.8053	−0.1532	0.5820	0.072*	
C11	0.7660 (3)	−0.03993 (13)	0.5220 (2)	0.0509 (5)	
H11	0.7733	−0.0187	0.6123	0.061*	
C12	0.7142 (4)	0.25279 (14)	0.6729 (3)	0.0694 (7)	
H12A	0.7253	0.2204	0.7557	0.104*	0.5
H12B	0.5916	0.2829	0.6741	0.104*	0.5
H12C	0.8274	0.2881	0.6712	0.104*	0.5
H12D	0.7043	0.3072	0.6449	0.104*	0.5
H12E	0.8379	0.2447	0.7266	0.104*	0.5
H12F	0.6021	0.2395	0.7295	0.104*	0.5
C13	0.8374 (4)	0.06195 (13)	0.0975 (2)	0.0552 (6)	
C14	0.7638 (4)	0.11009 (17)	−0.0244 (3)	0.0776 (8)	
H14A	0.6205	0.1038	−0.0371	0.116*	0.5
H14B	0.8285	0.0929	−0.1077	0.116*	0.5
H14C	0.7949	0.1647	−0.0073	0.116*	0.5
H14D	0.8754	0.1371	−0.0643	0.116*	0.5
H14E	0.6674	0.1481	0.0063	0.116*	0.5
H14F	0.7011	0.0762	−0.0942	0.116*	0.5
N1	0.7036 (3)	0.15221 (10)	0.33808 (19)	0.0611 (5)	
N2	0.6990 (3)	0.22223 (11)	0.4170 (2)	0.0669 (6)	
O1	0.6816 (2)	0.02180 (8)	0.15409 (14)	0.0548 (4)	
O2	1.0070 (2)	0.05640 (10)	0.14221 (17)	0.0666 (5)	
O4	0.7239 (2)	0.12238 (8)	0.56256 (14)	0.0491 (4)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.0587 (13)	0.0460 (12)	0.0541 (13)	0.0042 (10)	0.0026 (10)	−0.0013 (10)
C5	0.0451 (11)	0.0506 (11)	0.0391 (10)	0.0001 (8)	0.0021 (8)	0.0012 (9)
C6	0.0368 (10)	0.0470 (11)	0.0476 (11)	−0.0006 (8)	0.0021 (8)	0.0024 (9)
C7	0.0421 (10)	0.0490 (12)	0.0487 (12)	−0.0030 (8)	0.0011 (8)	0.0009 (9)
C8	0.0546 (12)	0.0531 (13)	0.0639 (14)	−0.0025 (10)	0.0026 (10)	−0.0103 (11)
C9	0.0547 (14)	0.0443 (12)	0.0853 (18)	0.0006 (10)	0.0070 (12)	0.0026 (12)
C10	0.0504 (12)	0.0543 (13)	0.0762 (16)	0.0013 (10)	0.0056 (11)	0.0214 (11)
C11	0.0452 (11)	0.0561 (13)	0.0517 (12)	−0.0011 (9)	0.0057 (9)	0.0100 (10)
C12	0.0863 (17)	0.0600 (14)	0.0617 (15)	0.0041 (13)	−0.0012 (12)	−0.0142 (11)
C13	0.0674 (15)	0.0549 (13)	0.0434 (11)	0.0016 (11)	0.0032 (10)	−0.0043 (9)
C14	0.0953 (19)	0.0802 (18)	0.0571 (14)	0.0043 (14)	0.0002 (13)	0.0150 (13)
N1	0.0915 (14)	0.0473 (10)	0.0446 (11)	0.0068 (9)	0.0045 (9)	0.0027 (8)
N2	0.0977 (15)	0.0453 (10)	0.0580 (12)	0.0072 (10)	0.0057 (10)	0.0011 (9)
O1	0.0577 (9)	0.0606 (9)	0.0456 (8)	−0.0032 (7)	−0.0046 (6)	0.0004 (7)
O2	0.0631 (11)	0.0777 (12)	0.0591 (10)	−0.0034 (8)	0.0038 (8)	0.0065 (8)
O4	0.0542 (8)	0.0504 (8)	0.0427 (8)	0.0029 (6)	0.0007 (6)	−0.0010 (6)

Geometric parameters (Å, º)

C3—N2	1.278 (3)	C12—H12A	0.9600
C3—O4	1.359 (2)	C12—H12B	0.9600
C3—C12	1.476 (3)	C12—H12C	0.9600
C5—N1	1.283 (3)	C12—H12D	0.9600
C5—O4	1.360 (2)	C12—H12E	0.9600
C5—C6	1.468 (3)	C12—H12F	0.9600
C6—C7	1.390 (3)	C13—O2	1.191 (3)
C6—C11	1.395 (3)	C13—O1	1.364 (3)
C7—C8	1.384 (3)	C13—C14	1.485 (3)
C7—O1	1.395 (2)	C14—H14A	0.9600
C8—C9	1.370 (3)	C14—H14B	0.9600
C8—H8	0.9300	C14—H14C	0.9600
C9—C10	1.380 (3)	C14—H14D	0.9600
C9—H9	0.9300	C14—H14E	0.9600
C10—C11	1.382 (3)	C14—H14F	0.9600
C10—H10	0.9300	N1—N2	1.404 (3)
C11—H11	0.9300		
N2—C3—O4	111.94 (18)	H12C—C12—H12E	56.3
N2—C3—C12	128.9 (2)	H12D—C12—H12E	109.5
O4—C3—C12	119.19 (19)	C3—C12—H12F	109.5
N1—C5—O4	112.05 (17)	H12A—C12—H12F	56.3
N1—C5—C6	130.60 (18)	H12B—C12—H12F	56.3
O4—C5—C6	117.34 (16)	H12C—C12—H12F	141.1
C7—C6—C11	117.89 (19)	H12D—C12—H12F	109.5
C7—C6—C5	122.15 (17)	H12E—C12—H12F	109.5

C11—C6—C5	119.94 (18)	O2—C13—O1	122.6 (2)
C8—C7—C6	121.16 (19)	O2—C13—C14	126.9 (2)
C8—C7—O1	117.97 (18)	O1—C13—C14	110.4 (2)
C6—C7—O1	120.73 (17)	C13—C14—H14A	109.5
C9—C8—C7	120.0 (2)	C13—C14—H14B	109.5
C9—C8—H8	120.0	H14A—C14—H14B	109.5
C7—C8—H8	120.0	C13—C14—H14C	109.5
C8—C9—C10	120.1 (2)	H14A—C14—H14C	109.5
C8—C9—H9	119.9	H14B—C14—H14C	109.5
C10—C9—H9	119.9	C13—C14—H14D	109.5
C9—C10—C11	120.1 (2)	H14A—C14—H14D	141.1
C9—C10—H10	120.0	H14B—C14—H14D	56.3
C11—C10—H10	120.0	H14C—C14—H14D	56.3
C10—C11—C6	120.8 (2)	C13—C14—H14E	109.5
C10—C11—H11	119.6	H14A—C14—H14E	56.3
C6—C11—H11	119.6	H14B—C14—H14E	141.1
C3—C12—H12A	109.5	H14C—C14—H14E	56.3
C3—C12—H12B	109.5	H14D—C14—H14E	109.5
H12A—C12—H12B	109.5	C13—C14—H14F	109.5
C3—C12—H12C	109.5	H14A—C14—H14F	56.3
H12A—C12—H12C	109.5	H14B—C14—H14F	56.3
H12B—C12—H12C	109.5	H14C—C14—H14F	141.1
C3—C12—H12D	109.5	H14D—C14—H14F	109.5
H12A—C12—H12D	141.1	H14E—C14—H14F	109.5
H12B—C12—H12D	56.3	C5—N1—N2	106.16 (17)
H12C—C12—H12D	56.3	C3—N2—N1	106.76 (17)
C3—C12—H12E	109.5	C13—O1—C7	117.22 (16)
H12A—C12—H12E	56.3	C3—O4—C5	103.10 (15)
H12B—C12—H12E	141.1		

C7—O1—C13—C14	−177.68 (18)	N1—C5—C6—C11	175.0 (2)
C13—O1—C7—C6	83.3 (2)	O4—C5—C6—C11	−3.4 (3)
C13—O1—C7—C8	−101.1 (2)	N1—C5—C6—C7	−3.5 (3)
C7—O1—C13—O2	3.3 (3)	C11—C6—C7—O1	175.59 (17)
C3—O4—C5—C6	178.30 (17)	C7—C6—C11—C10	−0.2 (3)
C5—O4—C3—N2	0.4 (2)	C11—C6—C7—C8	0.1 (3)
C3—O4—C5—N1	−0.4 (2)	C5—C6—C7—C8	178.61 (19)
C5—O4—C3—C12	−179.60 (19)	C5—C6—C7—O1	−5.9 (3)
C5—N1—N2—C3	0.0 (2)	C5—C6—C11—C10	−178.75 (19)
N2—N1—C5—O4	0.2 (2)	C6—C7—C8—C9	−0.2 (3)
N2—N1—C5—C6	−178.2 (2)	O1—C7—C8—C9	−175.85 (18)
N1—N2—C3—O4	−0.2 (2)	C7—C8—C9—C10	0.5 (3)
N1—N2—C3—C12	179.7 (2)	C8—C9—C10—C11	−0.6 (3)
O4—C5—C6—C7	178.11 (18)	C9—C10—C11—C6	0.5 (3)