

Methyl (4-oxo-1-phenyl-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-5-yl)acetate

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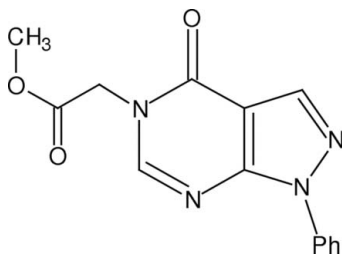
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.035; wR factor = 0.096; data-to-parameter ratio = 15.2.

The title compound, $\text{C}_{14}\text{H}_{12}\text{N}_4\text{O}_3$, a pyrazolopyrimidine derivative, displays normal geometrical parameters. The dihedral angle between the mean planes of the pyrazolopyrimidine unit and the phenyl ring is $26.14(4)^\circ$. The non-H atoms of the ester side chain are coplanar (r.m.s. deviation = 0.009 Å) and this plane is almost perpendicular [dihedral angle = $84.31(4)^\circ$] to the central ring system.

Related literature

For related structures, see: Wen *et al.* (2004); Oliveira-Campos *et al.* (2006) and Portilla *et al.* (2005). For background literature, see: Garg *et al.* (1990); El-Feky & Abd El-Samii (1996); Ismail, *et al.* (2003); Devesa, *et al.* (2004) and Russo *et al.* (1993).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{12}\text{N}_4\text{O}_3$
 $M_r = 284.28$
 Triclinic, $P\bar{1}$
 $a = 6.8628(8)$ Å
 $b = 7.6128(9)$ Å
 $c = 12.4949(16)$ Å
 $\alpha = 87.036(10)^\circ$
 $\beta = 89.608(11)^\circ$
 $\gamma = 79.973(8)^\circ$
 $V = 641.97(13)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 173(2)$ K
 $0.45 \times 0.43 \times 0.42$ mm

Data collection

Stoe IPDSII two-circle diffractometer
 Absorption correction: none
 6143 measured reflections
 2914 independent reflections
 2601 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.096$
 $S = 1.02$
 2914 reflections
 192 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: HB2372).

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supplementary materials

Acta Cryst. (2007). E63, o2566 [doi:10.1107/S1600536807018934]

Methyl (4-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazolo[3,4-*d*]pyrimidin-5-yl)acetate

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Comment

Pyrazolo[3,4-*d*]pyrimidines and their derivatives are of interest as potential bioactive molecules. Various pyrazolopyrimidine derivatives are reported to have antileishmanial, antihypertensive, antibacterial and antifungal, antiangiogenic, antiinflammatory and analgesic activities. The title compound, a new pyrazolopyrimidine derivative, (I), C₁₄H₁₂N₄O₃, has been synthesized and its crystal structure determined.

Experimental

4-Hydroxy-1-phenyl pyrazolo[3,4-*d*]pyrimidine (21.2 g, 0.1 mol) in 180 ml acetone was stirred with anhydrous potassium carbonate (16.5 g, 0.12 mol) at room temperature and methyl chloroacetate (12.2 g, 0.1 mol) was added to it drop-wise. The reaction mixture was then refluxed for 8 h. Progress of the reaction was monitored by TLC. The acetone was distilled out and the residue was diluted with 250 ml water. The solid obtained was filtered, washed with water and then recrystallized from methanol to obtain the title compound as colourless needles (Yield: 95%; m.p.: 421-424 K). Crystals of (I) suitable for X-ray diffraction were obtained from acetone by slow evaporation. Analysis for (I), C₁₄H₁₂N₄O₃: Found (Calculated): C: 59.01 (59.15); H: 4.11 (4.25); N: 19.62% (19.71%). ¹H-NMR (400 MHz, CDCl₃): δ 3.78 (s, 3H, -CH₃), 4.73 (s, 2H, -CH₂), 7.34 (t, 1H, ArH), 7.48 (t, 2H, ArH), 7.94 (s, 1H, ArH), 7.99 (d (J = 6.08), 1H, ArH), 8.23 (s, 1H, ArH).

Refinement

The H atoms were found in a difference map, repositioned in idealised locations (C—H = 0.95-0.99 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. The methyl group was allowed to rotate but not to tip to best fit the electron density.

Figures

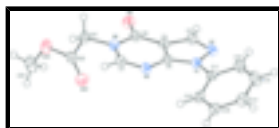


Fig. 1. Perspective view of (I) with the atom numbering; displacement ellipsoids are at the 50% probability level (arbitrary spheres for the H atoms).

Methyl (4-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazolo[3,4-*d*]pyrimidin-5-yl)acetate

Crystal data

C₁₄H₁₂N₄O₃

$M_r = 284.28$

Triclinic, *P* $\bar{1}$

$Z = 2$

$F_{000} = 296$

$D_x = 1.471 \text{ Mg m}^{-3}$

supplementary materials

Hall symbol: -P 1

$a = 6.8628$ (8) Å

$b = 7.6128$ (9) Å

$c = 12.4949$ (16) Å

$\alpha = 87.036$ (10)°

$\beta = 89.608$ (11)°

$\gamma = 79.973$ (8)°

$V = 641.97$ (13) Å³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5143 reflections

$\theta = 3.9$ – 26.8 °

$\mu = 0.11$ mm⁻¹

$T = 173$ (2) K

Block, colourless

$0.45 \times 0.43 \times 0.42$ mm

Data collection

Stoe IPDSII two-circle diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 173$ (2) K

ω scans

Absorption correction: none

6143 measured reflections

2914 independent reflections

2601 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\text{max}} = 27.6$ °

$\theta_{\text{min}} = 3.7$ °

$h = -8 \rightarrow 8$

$k = -9 \rightarrow 9$

$l = -16 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.096$

$S = 1.02$

2914 reflections

192 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.1857P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.28$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Extinction correction: SHELXL97,

$F_c^* = kFc[1 + 0.001x Fc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.070 (7)

Special details

Experimental ;

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|---------------|---------------|----------------------------------|
| N1 | 0.39377 (13) | 0.15427 (12) | 0.60302 (7) | 0.0202 (2) |
| N2 | 0.59660 (13) | 0.14301 (13) | 0.61111 (7) | 0.0234 (2) |
| C3 | 0.65154 (16) | 0.22729 (14) | 0.52324 (9) | 0.0228 (2) |
| H3 | 0.7840 | 0.2402 | 0.5073 | 0.027* |
| C4 | 0.48698 (15) | 0.29526 (14) | 0.45657 (8) | 0.0207 (2) |
| C5 | 0.32439 (15) | 0.24664 (14) | 0.51033 (8) | 0.0193 (2) |
| N6 | 0.13029 (13) | 0.28745 (13) | 0.47750 (7) | 0.0228 (2) |
| C7 | 0.10838 (16) | 0.38329 (15) | 0.38733 (9) | 0.0237 (2) |
| H7 | -0.0225 | 0.4156 | 0.3599 | 0.028* |
| N8 | 0.25607 (14) | 0.44203 (13) | 0.32814 (7) | 0.0233 (2) |
| C9 | 0.45997 (16) | 0.40085 (14) | 0.35729 (8) | 0.0224 (2) |
| O9 | 0.58579 (13) | 0.45707 (12) | 0.30136 (7) | 0.0298 (2) |
| C11 | 0.28917 (16) | 0.08388 (14) | 0.69005 (8) | 0.0209 (2) |
| C12 | 0.37358 (19) | 0.06459 (19) | 0.79214 (10) | 0.0332 (3) |
| H12 | 0.4986 | 0.0979 | 0.8036 | 0.040* |
| C13 | 0.2726 (2) | -0.0040 (2) | 0.87694 (10) | 0.0412 (3) |
| H13 | 0.3298 | -0.0178 | 0.9465 | 0.049* |
| C14 | 0.0892 (2) | -0.05258 (17) | 0.86134 (10) | 0.0320 (3) |
| H14 | 0.0208 | -0.0982 | 0.9199 | 0.038* |
| C15 | 0.00682 (17) | -0.03376 (15) | 0.75916 (9) | 0.0264 (2) |
| H15 | -0.1185 | -0.0668 | 0.7480 | 0.032* |
| C16 | 0.10647 (16) | 0.03323 (15) | 0.67283 (9) | 0.0239 (2) |
| H16 | 0.0505 | 0.0443 | 0.6030 | 0.029* |
| C21 | 0.20561 (18) | 0.55468 (15) | 0.23041 (9) | 0.0269 (2) |
| H21A | 0.2833 | 0.6529 | 0.2277 | 0.032* |
| H21B | 0.0636 | 0.6085 | 0.2319 | 0.032* |
| C22 | 0.24787 (16) | 0.44799 (16) | 0.13065 (9) | 0.0241 (2) |
| O22 | 0.28503 (14) | 0.28799 (12) | 0.12993 (7) | 0.0346 (2) |
| O23 | 0.23286 (13) | 0.55953 (12) | 0.04324 (6) | 0.0327 (2) |
| C23 | 0.2652 (2) | 0.4720 (2) | -0.05810 (10) | 0.0403 (3) |
| H23A | 0.3964 | 0.3966 | -0.0576 | 0.061* |
| H23B | 0.2571 | 0.5626 | -0.1173 | 0.061* |
| H23C | 0.1638 | 0.3980 | -0.0676 | 0.061* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|------------|------------|------------|-------------|------------|-------------|
| N1 | 0.0177 (4) | 0.0235 (4) | 0.0201 (4) | -0.0055 (3) | 0.0006 (3) | 0.0001 (3) |
| N2 | 0.0173 (4) | 0.0279 (5) | 0.0256 (5) | -0.0057 (3) | 0.0007 (3) | -0.0013 (4) |

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| | | | | | | |
|-----|------------|------------|------------|-------------|-------------|-------------|
| C3 | 0.0193 (5) | 0.0253 (5) | 0.0250 (5) | -0.0063 (4) | 0.0032 (4) | -0.0035 (4) |
| C4 | 0.0207 (5) | 0.0222 (5) | 0.0207 (5) | -0.0070 (4) | 0.0042 (4) | -0.0035 (4) |
| C5 | 0.0203 (5) | 0.0203 (5) | 0.0183 (5) | -0.0060 (4) | 0.0023 (4) | -0.0027 (4) |
| N6 | 0.0199 (4) | 0.0281 (5) | 0.0210 (4) | -0.0061 (3) | 0.0003 (3) | 0.0002 (3) |
| C7 | 0.0220 (5) | 0.0282 (5) | 0.0215 (5) | -0.0061 (4) | 0.0005 (4) | -0.0012 (4) |
| N8 | 0.0272 (5) | 0.0262 (5) | 0.0172 (4) | -0.0068 (4) | 0.0014 (3) | 0.0007 (3) |
| C9 | 0.0254 (5) | 0.0234 (5) | 0.0198 (5) | -0.0073 (4) | 0.0049 (4) | -0.0043 (4) |
| O9 | 0.0311 (4) | 0.0340 (5) | 0.0262 (4) | -0.0118 (3) | 0.0097 (3) | 0.0009 (3) |
| C11 | 0.0229 (5) | 0.0205 (5) | 0.0194 (5) | -0.0048 (4) | 0.0030 (4) | -0.0001 (4) |
| C12 | 0.0319 (6) | 0.0483 (7) | 0.0231 (6) | -0.0183 (5) | -0.0025 (5) | 0.0032 (5) |
| C13 | 0.0460 (8) | 0.0622 (9) | 0.0196 (6) | -0.0232 (7) | -0.0031 (5) | 0.0061 (6) |
| C14 | 0.0373 (7) | 0.0366 (6) | 0.0238 (6) | -0.0125 (5) | 0.0074 (5) | 0.0031 (5) |
| C15 | 0.0248 (5) | 0.0268 (6) | 0.0283 (6) | -0.0074 (4) | 0.0046 (4) | 0.0014 (4) |
| C16 | 0.0235 (5) | 0.0268 (5) | 0.0218 (5) | -0.0063 (4) | 0.0004 (4) | 0.0011 (4) |
| C21 | 0.0340 (6) | 0.0269 (5) | 0.0196 (5) | -0.0062 (5) | 0.0008 (4) | 0.0023 (4) |
| C22 | 0.0211 (5) | 0.0324 (6) | 0.0202 (5) | -0.0094 (4) | 0.0017 (4) | 0.0021 (4) |
| O22 | 0.0459 (5) | 0.0322 (5) | 0.0276 (4) | -0.0115 (4) | 0.0041 (4) | -0.0029 (3) |
| O23 | 0.0375 (5) | 0.0406 (5) | 0.0188 (4) | -0.0053 (4) | 0.0035 (3) | 0.0053 (3) |
| C23 | 0.0387 (7) | 0.0624 (9) | 0.0191 (6) | -0.0070 (6) | 0.0040 (5) | -0.0018 (5) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|-------------|-------------|
| N1—C5 | 1.3672 (13) | C12—H12 | 0.9500 |
| N1—N2 | 1.3838 (12) | C13—C14 | 1.3898 (19) |
| N1—C11 | 1.4311 (13) | C13—H13 | 0.9500 |
| N2—C3 | 1.3286 (14) | C14—C15 | 1.3904 (17) |
| C3—C4 | 1.4148 (15) | C14—H14 | 0.9500 |
| C3—H3 | 0.9500 | C15—C16 | 1.3949 (15) |
| C4—C5 | 1.3933 (14) | C15—H15 | 0.9500 |
| C4—C9 | 1.4379 (15) | C16—H16 | 0.9500 |
| C5—N6 | 1.3745 (13) | C21—C22 | 1.5216 (16) |
| N6—C7 | 1.3052 (14) | C21—H21A | 0.9900 |
| C7—N8 | 1.3739 (14) | C21—H21B | 0.9900 |
| C7—H7 | 0.9500 | C22—O22 | 1.2007 (15) |
| N8—C9 | 1.4253 (15) | C22—O23 | 1.3415 (13) |
| N8—C21 | 1.4629 (14) | O23—C23 | 1.4591 (16) |
| C9—O9 | 1.2274 (13) | C23—H23A | 0.9800 |
| C11—C12 | 1.3947 (16) | C23—H23B | 0.9800 |
| C11—C16 | 1.3956 (15) | C23—H23C | 0.9800 |
| C12—C13 | 1.3908 (17) | | |
| C5—N1—N2 | 110.59 (8) | C14—C13—C12 | 120.96 (11) |
| C5—N1—C11 | 130.25 (9) | C14—C13—H13 | 119.5 |
| N2—N1—C11 | 119.01 (8) | C12—C13—H13 | 119.5 |
| C3—N2—N1 | 106.00 (9) | C13—C14—C15 | 119.36 (11) |
| N2—C3—C4 | 111.14 (9) | C13—C14—H14 | 120.3 |
| N2—C3—H3 | 124.4 | C15—C14—H14 | 120.3 |
| C4—C3—H3 | 124.4 | C14—C15—C16 | 120.59 (11) |
| C5—C4—C3 | 105.19 (9) | C14—C15—H15 | 119.7 |
| C5—C4—C9 | 120.20 (10) | C16—C15—H15 | 119.7 |

| | | | |
|--------------|--------------|-----------------|--------------|
| C3—C4—C9 | 134.53 (10) | C15—C16—C11 | 119.38 (10) |
| N1—C5—N6 | 126.48 (9) | C15—C16—H16 | 120.3 |
| N1—C5—C4 | 107.09 (9) | C11—C16—H16 | 120.3 |
| N6—C5—C4 | 126.42 (10) | N8—C21—C22 | 111.45 (9) |
| C7—N6—C5 | 112.58 (9) | N8—C21—H21A | 109.3 |
| N6—C7—N8 | 126.36 (10) | C22—C21—H21A | 109.3 |
| N6—C7—H7 | 116.8 | N8—C21—H21B | 109.3 |
| N8—C7—H7 | 116.8 | C22—C21—H21B | 109.3 |
| C7—N8—C9 | 123.41 (9) | H21A—C21—H21B | 108.0 |
| C7—N8—C21 | 119.58 (10) | O22—C22—O23 | 125.04 (11) |
| C9—N8—C21 | 117.01 (9) | O22—C22—C21 | 125.21 (10) |
| O9—C9—N8 | 120.64 (10) | O23—C22—C21 | 109.73 (10) |
| O9—C9—C4 | 128.34 (11) | C22—O23—C23 | 114.78 (10) |
| N8—C9—C4 | 111.00 (9) | O23—C23—H23A | 109.5 |
| C12—C11—C16 | 120.46 (10) | O23—C23—H23B | 109.5 |
| C12—C11—N1 | 119.03 (10) | H23A—C23—H23B | 109.5 |
| C16—C11—N1 | 120.51 (9) | O23—C23—H23C | 109.5 |
| C13—C12—C11 | 119.24 (11) | H23A—C23—H23C | 109.5 |
| C13—C12—H12 | 120.4 | H23B—C23—H23C | 109.5 |
| C11—C12—H12 | 120.4 | | |
| C5—N1—N2—C3 | -0.39 (12) | C5—C4—C9—O9 | 178.62 (11) |
| C11—N1—N2—C3 | -176.28 (9) | C3—C4—C9—O9 | 2.3 (2) |
| N1—N2—C3—C4 | 0.16 (12) | C5—C4—C9—N8 | 0.20 (14) |
| N2—C3—C4—C5 | 0.12 (12) | C3—C4—C9—N8 | -176.09 (11) |
| N2—C3—C4—C9 | 176.79 (11) | C5—N1—C11—C12 | -152.52 (12) |
| N2—N1—C5—N6 | -178.17 (10) | N2—N1—C11—C12 | 22.44 (15) |
| C11—N1—C5—N6 | -2.88 (18) | C5—N1—C11—C16 | 28.25 (17) |
| N2—N1—C5—C4 | 0.47 (12) | N2—N1—C11—C16 | -156.79 (10) |
| C11—N1—C5—C4 | 175.76 (10) | C16—C11—C12—C13 | -0.7 (2) |
| C3—C4—C5—N1 | -0.35 (11) | N1—C11—C12—C13 | -179.91 (12) |
| C9—C4—C5—N1 | -177.61 (9) | C11—C12—C13—C14 | -0.3 (2) |
| C3—C4—C5—N6 | 178.29 (10) | C12—C13—C14—C15 | 0.6 (2) |
| C9—C4—C5—N6 | 1.03 (16) | C13—C14—C15—C16 | 0.0 (2) |
| N1—C5—N6—C7 | 177.41 (10) | C14—C15—C16—C11 | -0.90 (18) |
| C4—C5—N6—C7 | -0.97 (16) | C12—C11—C16—C15 | 1.26 (17) |
| C5—N6—C7—N8 | -0.33 (16) | N1—C11—C16—C15 | -179.52 (10) |
| N6—C7—N8—C9 | 1.61 (18) | C7—N8—C21—C22 | -101.82 (12) |
| N6—C7—N8—C21 | -177.63 (11) | C9—N8—C21—C22 | 78.89 (12) |
| C7—N8—C9—O9 | -179.96 (10) | N8—C21—C22—O22 | 12.05 (16) |
| C21—N8—C9—O9 | -0.71 (15) | N8—C21—C22—O23 | -169.38 (9) |
| C7—N8—C9—C4 | -1.40 (14) | O22—C22—O23—C23 | 0.15 (17) |
| C21—N8—C9—C4 | 177.86 (9) | C21—C22—O23—C23 | -178.43 (10) |

Fig. 1

