

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2-(*o*-Tolyloxy)pyrimidine

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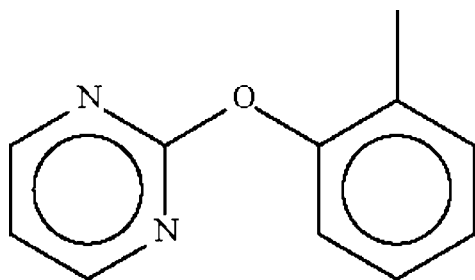
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Received 7 July 2009; accepted 8 July 2009

Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.033; wR factor = 0.088; data-to-parameter ratio = 9.1.

The title compound, $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}$, crystallizes with two molecules in the asymmetric unit. The angle at the ether O atom is widened to 118.13 (15)° [117.89 (16)° for the second molecule in the asymmetric unit]; the six-membered rings subtend a dihedral angle of 84.3 (1)° [87.4 (1)° in the second molecule].

Related literature

For 2-phenoxy pyrimidine, see: Shah Bakhtiar *et al.* (2009).

Experimental

Crystal data

$\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}$	$V = 1956.16$ (8) Å ³
$M_r = 186.21$	$Z = 8$
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
$a = 7.5197$ (2) Å	$\mu = 0.08$ mm ⁻¹
$b = 12.7997$ (3) Å	$T = 153$ K
$c = 20.3238$ (4) Å	$0.35 \times 0.25 \times 0.15$ mm

Data collection

Bruker SMART APEX diffractometer	2317 independent reflections
Absorption correction: none	2030 reflections with $I > 2\sigma(I)$
12792 measured reflections	$R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$	1 restraint
$wR(F^2) = 0.088$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.16$ e Å ⁻³
2317 reflections	$\Delta\rho_{\text{min}} = -0.19$ e Å ⁻³
255 parameters	

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2009).

We thank the University of Malaya (FP047/2008 C, RG027/09AFR) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2995).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
 Bruker (2008). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Shah Bakhtiar, N., Abdullah, Z. & Ng, S. W. (2009). *Acta Cryst.* **E65**, o114.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Westrip, S. P. (2009). *pubCIF*. In preparation.

supporting information

Acta Cryst. (2009). E65, o1880 [doi:10.1107/S1600536809026609]

2-(*o*-Tolyloxy)pyrimidine

Nasir Shah Bakhtiar, Zanariah Abdullah and Seik Weng Ng

S1. Experimental

o-Cresol (2.16 g, 20 mmol) and sodium hydroxide (0.80 g, 20 mmol) were dissolved in water (50 ml) and to the solution was added 2-chloropyrimidine (2.30 g, 20 mmol) dissolved in THF (50 ml). The mixture was heated for 4 h. Water was added and the organic phase extracted with chloroform. The chloroform solution was dried over sodium sulfate; slow evaporation led to the formation of colorless crystals.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95–0.98 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to 1.2–1.5 $U(\text{C})$.

In the absence of anomalous scatterers, 2119 Friedel pairs were merged. The absolute structure was arbitrarily set.

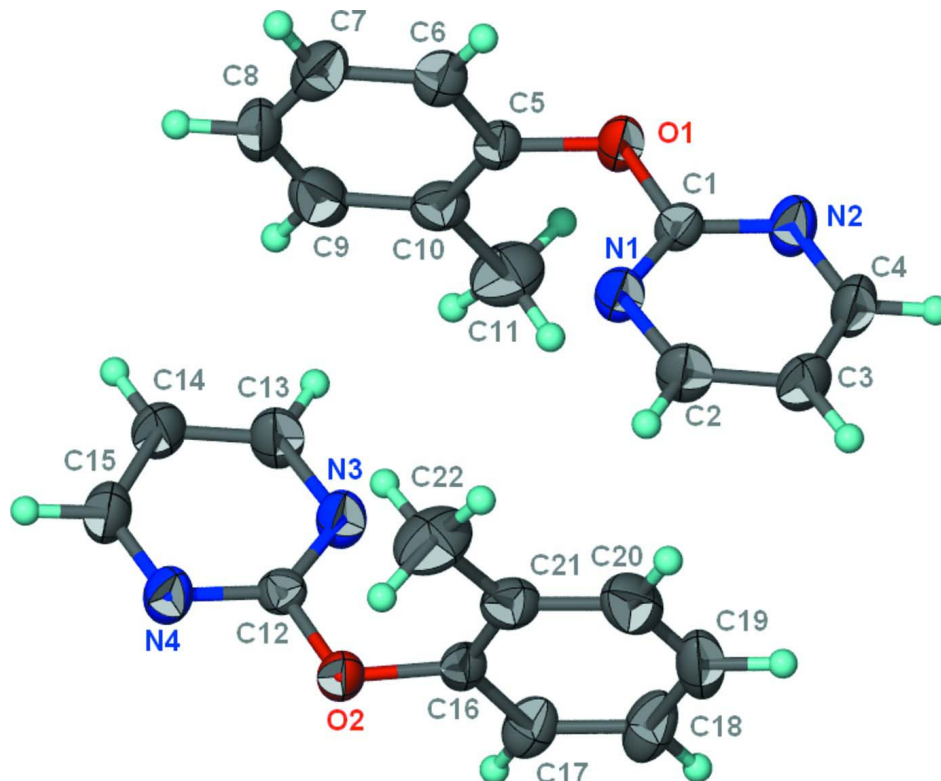


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-(*o*-Tolyloxy)pyrimidine*Crystal data*C₁₁H₁₀N₂O $M_r = 186.21$ Orthorhombic, *Pca*2₁

Hall symbol: P 2c -2ac

 $a = 7.5197$ (2) Å $b = 12.7997$ (3) Å $c = 20.3238$ (4) Å $V = 1956.16$ (8) Å³ $Z = 8$ $F(000) = 784$ $D_x = 1.265$ Mg m⁻³Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 3906 reflections

 $\theta = 2.6$ – 27.9° $\mu = 0.08$ mm⁻¹ $T = 153$ K

Block, colorless

 $0.35 \times 0.25 \times 0.15$ mm*Data collection*

Bruker SMART APEX

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω scans

12792 measured reflections

2317 independent reflections

2030 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.028$ $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.6^\circ$ $h = -9 \rightarrow 9$ $k = -16 \rightarrow 16$ $l = -26 \rightarrow 26$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.088$ $S = 1.02$

2317 reflections

255 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

 $w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.3519P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.09137 (18)	0.69839 (11)	0.50102 (8)	0.0294 (3)
O2	0.3463 (2)	0.79763 (11)	0.83583 (8)	0.0288 (3)
N1	0.3704 (2)	0.76815 (13)	0.51731 (9)	0.0290 (4)
N2	0.3222 (2)	0.59497 (13)	0.47797 (10)	0.0346 (4)
N3	0.0668 (3)	0.73277 (14)	0.81493 (10)	0.0311 (4)
N4	0.1165 (3)	0.90210 (14)	0.85951 (10)	0.0342 (4)
C1	0.2716 (3)	0.68835 (14)	0.49926 (10)	0.0240 (4)
C2	0.5457 (3)	0.75182 (17)	0.51316 (13)	0.0346 (5)
H2	0.6241	0.8068	0.5252	0.041*
C3	0.6173 (3)	0.65849 (18)	0.49217 (13)	0.0369 (5)
H3	0.7421	0.6478	0.4895	0.044*
C4	0.4976 (3)	0.58168 (19)	0.47530 (14)	0.0393 (6)
H4	0.5424	0.5160	0.4611	0.047*
C5	0.0193 (3)	0.78821 (16)	0.53078 (11)	0.0260 (4)
C6	-0.0168 (3)	0.87417 (16)	0.49211 (12)	0.0302 (5)

H6	0.0168	0.8751	0.4471	0.036*
C7	-0.1029 (3)	0.95922 (17)	0.51989 (13)	0.0369 (5)
H7	-0.1291	1.0191	0.4940	0.044*
C8	-0.1500 (3)	0.95613 (18)	0.58534 (14)	0.0400 (6)
H8	-0.2097	1.0140	0.6046	0.048*
C9	-0.1111 (3)	0.8691 (2)	0.62345 (13)	0.0419 (6)
H9	-0.1435	0.8687	0.6686	0.050*
C10	-0.0255 (3)	0.78224 (18)	0.59682 (11)	0.0318 (5)
C11	0.0132 (4)	0.6853 (2)	0.63601 (14)	0.0484 (7)
H11A	0.1420	0.6738	0.6377	0.073*
H11B	-0.0442	0.6251	0.6151	0.073*
H11C	-0.0328	0.6936	0.6808	0.073*
C12	0.1667 (3)	0.81024 (15)	0.83622 (10)	0.0239 (4)
C13	-0.1090 (3)	0.75137 (18)	0.81651 (12)	0.0362 (5)
H13	-0.1879	0.6982	0.8019	0.043*
C14	-0.1789 (3)	0.84386 (17)	0.83828 (12)	0.0360 (5)
H14	-0.3034	0.8565	0.8383	0.043*
C15	-0.0596 (3)	0.91746 (18)	0.86010 (14)	0.0392 (6)
H15	-0.1039	0.9820	0.8763	0.047*
C16	0.4168 (3)	0.71305 (15)	0.79991 (10)	0.0254 (4)
C17	0.4576 (3)	0.62233 (17)	0.83289 (13)	0.0337 (5)
H17	0.4291	0.6148	0.8782	0.040*
C18	0.5409 (3)	0.54212 (18)	0.79914 (15)	0.0417 (6)
H18	0.5700	0.4789	0.8211	0.050*
C19	0.5813 (3)	0.5547 (2)	0.73329 (15)	0.0445 (6)
H19	0.6388	0.4999	0.7100	0.053*
C20	0.5387 (3)	0.6461 (2)	0.70137 (13)	0.0433 (6)
H20	0.5663	0.6530	0.6560	0.052*
C21	0.4562 (3)	0.72886 (19)	0.73387 (12)	0.0328 (5)
C22	0.4127 (4)	0.8309 (2)	0.70067 (14)	0.0513 (7)
H22A	0.4773	0.8877	0.7225	0.077*
H22B	0.2845	0.8439	0.7036	0.077*
H22C	0.4481	0.8275	0.6543	0.077*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0202 (8)	0.0232 (7)	0.0447 (9)	-0.0012 (6)	-0.0002 (6)	-0.0071 (6)
O2	0.0207 (8)	0.0268 (7)	0.0389 (8)	0.0008 (6)	-0.0035 (6)	-0.0081 (6)
N1	0.0227 (9)	0.0239 (8)	0.0404 (10)	-0.0021 (7)	-0.0004 (8)	-0.0044 (8)
N2	0.0261 (10)	0.0239 (9)	0.0540 (12)	0.0003 (7)	-0.0015 (9)	-0.0096 (8)
N3	0.0246 (10)	0.0255 (9)	0.0433 (11)	-0.0027 (7)	0.0012 (8)	-0.0061 (8)
N4	0.0274 (11)	0.0249 (9)	0.0503 (11)	0.0003 (7)	-0.0039 (9)	-0.0087 (9)
C1	0.0213 (10)	0.0214 (9)	0.0292 (10)	-0.0003 (7)	-0.0012 (8)	0.0014 (8)
C2	0.0232 (12)	0.0315 (12)	0.0490 (14)	-0.0067 (9)	-0.0006 (10)	-0.0074 (11)
C3	0.0199 (11)	0.0410 (13)	0.0499 (13)	0.0042 (9)	-0.0008 (10)	-0.0085 (11)
C4	0.0296 (12)	0.0316 (12)	0.0567 (15)	0.0092 (9)	-0.0024 (11)	-0.0134 (11)
C5	0.0183 (10)	0.0241 (10)	0.0357 (11)	-0.0007 (7)	-0.0015 (8)	-0.0041 (8)

C6	0.0259 (11)	0.0275 (10)	0.0373 (11)	-0.0023 (8)	0.0013 (9)	-0.0001 (9)
C7	0.0269 (12)	0.0251 (10)	0.0587 (15)	-0.0006 (8)	-0.0047 (11)	-0.0002 (10)
C8	0.0259 (12)	0.0328 (12)	0.0614 (15)	0.0031 (9)	-0.0020 (11)	-0.0210 (11)
C9	0.0304 (13)	0.0549 (15)	0.0403 (13)	-0.0003 (11)	0.0010 (10)	-0.0152 (12)
C10	0.0232 (11)	0.0375 (12)	0.0346 (12)	-0.0014 (9)	-0.0031 (8)	-0.0004 (10)
C11	0.0465 (16)	0.0536 (16)	0.0450 (14)	0.0039 (12)	-0.0021 (12)	0.0111 (12)
C12	0.0229 (11)	0.0226 (9)	0.0260 (9)	-0.0012 (8)	-0.0022 (8)	0.0010 (8)
C13	0.0246 (12)	0.0349 (12)	0.0492 (13)	-0.0044 (9)	0.0013 (10)	-0.0113 (11)
C14	0.0226 (12)	0.0401 (12)	0.0453 (12)	0.0021 (9)	-0.0006 (10)	-0.0090 (11)
C15	0.0315 (13)	0.0321 (12)	0.0541 (14)	0.0064 (9)	-0.0028 (11)	-0.0128 (11)
C16	0.0175 (10)	0.0240 (10)	0.0346 (11)	-0.0008 (8)	-0.0011 (8)	-0.0047 (8)
C17	0.0271 (12)	0.0289 (11)	0.0452 (13)	-0.0003 (9)	0.0037 (10)	0.0030 (10)
C18	0.0302 (13)	0.0240 (11)	0.0709 (17)	0.0006 (9)	0.0035 (12)	-0.0010 (11)
C19	0.0294 (13)	0.0401 (13)	0.0640 (16)	0.0009 (10)	0.0028 (12)	-0.0244 (12)
C20	0.0332 (14)	0.0600 (17)	0.0368 (12)	0.0010 (12)	0.0037 (10)	-0.0129 (12)
C21	0.0255 (12)	0.0375 (12)	0.0353 (11)	-0.0013 (9)	-0.0024 (9)	-0.0001 (10)
C22	0.0511 (17)	0.0592 (18)	0.0435 (14)	0.0078 (14)	0.0015 (13)	0.0192 (13)

Geometric parameters (Å, °)

O1—C1	1.362 (2)	C9—C10	1.394 (3)
O1—C5	1.408 (2)	C9—H9	0.9500
O2—C12	1.360 (2)	C10—C11	1.503 (4)
O2—C16	1.409 (2)	C11—H11A	0.9800
N1—C1	1.315 (3)	C11—H11B	0.9800
N1—C2	1.337 (3)	C11—H11C	0.9800
N2—C4	1.332 (3)	C13—C14	1.369 (3)
N2—C1	1.327 (2)	C13—H13	0.9500
N3—C12	1.317 (3)	C14—C15	1.375 (3)
N3—C13	1.343 (3)	C14—H14	0.9500
N4—C12	1.323 (3)	C15—H15	0.9500
N4—C15	1.339 (3)	C16—C17	1.375 (3)
C2—C3	1.378 (3)	C16—C21	1.389 (3)
C2—H2	0.9500	C17—C18	1.384 (3)
C3—C4	1.376 (3)	C17—H17	0.9500
C3—H3	0.9500	C18—C19	1.382 (4)
C4—H4	0.9500	C18—H18	0.9500
C5—C6	1.379 (3)	C19—C20	1.376 (4)
C5—C10	1.386 (3)	C19—H19	0.9500
C6—C7	1.387 (3)	C20—C21	1.394 (3)
C6—H6	0.9500	C20—H20	0.9500
C7—C8	1.377 (4)	C21—C22	1.506 (3)
C7—H7	0.9500	C22—H22A	0.9800
C8—C9	1.388 (4)	C22—H22B	0.9800
C8—H8	0.9500	C22—H22C	0.9800
C1—O1—C5	118.13 (15)	C10—C11—H11C	109.5
C12—O2—C16	117.89 (16)	H11A—C11—H11C	109.5

C1—N1—C2	114.70 (18)	H11B—C11—H11C	109.5
C4—N2—C1	114.36 (19)	N3—C12—N4	128.6 (2)
C12—N3—C13	114.84 (19)	N3—C12—O2	118.38 (18)
C12—N4—C15	114.59 (19)	N4—C12—O2	113.02 (17)
N1—C1—N2	128.94 (19)	N3—C13—C14	122.6 (2)
N1—C1—O1	118.79 (17)	N3—C13—H13	118.7
N2—C1—O1	112.27 (17)	C14—C13—H13	118.7
N1—C2—C3	122.7 (2)	C13—C14—C15	116.5 (2)
N1—C2—H2	118.6	C13—C14—H14	121.8
C3—C2—H2	118.6	C15—C14—H14	121.8
C2—C3—C4	116.2 (2)	N4—C15—C14	122.8 (2)
C2—C3—H3	121.9	N4—C15—H15	118.6
C4—C3—H3	121.9	C14—C15—H15	118.6
N2—C4—C3	123.1 (2)	C17—C16—C21	123.1 (2)
N2—C4—H4	118.4	C17—C16—O2	118.68 (19)
C3—C4—H4	118.4	C21—C16—O2	117.95 (19)
C6—C5—C10	123.2 (2)	C16—C17—C18	119.0 (2)
C6—C5—O1	118.85 (19)	C16—C17—H17	120.5
C10—C5—O1	117.69 (19)	C18—C17—H17	120.5
C5—C6—C7	119.1 (2)	C17—C18—C19	119.6 (2)
C5—C6—H6	120.4	C17—C18—H18	120.2
C7—C6—H6	120.4	C19—C18—H18	120.2
C8—C7—C6	119.4 (2)	C20—C19—C18	120.3 (2)
C8—C7—H7	120.3	C20—C19—H19	119.9
C6—C7—H7	120.3	C18—C19—H19	119.9
C7—C8—C9	120.5 (2)	C19—C20—C21	121.8 (2)
C7—C8—H8	119.7	C19—C20—H20	119.1
C9—C8—H8	119.7	C21—C20—H20	119.1
C8—C9—C10	121.4 (2)	C16—C21—C20	116.2 (2)
C8—C9—H9	119.3	C16—C21—C22	120.9 (2)
C10—C9—H9	119.3	C20—C21—C22	122.9 (2)
C5—C10—C9	116.4 (2)	C21—C22—H22A	109.5
C5—C10—C11	120.8 (2)	C21—C22—H22B	109.5
C9—C10—C11	122.8 (2)	H22A—C22—H22B	109.5
C10—C11—H11A	109.5	C21—C22—H22C	109.5
C10—C11—H11B	109.5	H22A—C22—H22C	109.5
H11A—C11—H11B	109.5	H22B—C22—H22C	109.5
C2—N1—C1—N2	0.2 (3)	C13—N3—C12—N4	1.1 (3)
C2—N1—C1—O1	-179.1 (2)	C13—N3—C12—O2	-179.6 (2)
C4—N2—C1—N1	0.5 (4)	C15—N4—C12—N3	-1.2 (3)
C4—N2—C1—O1	179.9 (2)	C15—N4—C12—O2	179.5 (2)
C5—O1—C1—N1	-8.8 (3)	C16—O2—C12—N3	13.5 (3)
C5—O1—C1—N2	171.72 (19)	C16—O2—C12—N4	-167.07 (18)
C1—N1—C2—C3	-0.5 (4)	C12—N3—C13—C14	0.3 (3)
N1—C2—C3—C4	0.1 (4)	N3—C13—C14—C15	-1.3 (4)
C1—N2—C4—C3	-0.9 (4)	C12—N4—C15—C14	0.0 (4)
C2—C3—C4—N2	0.7 (4)	C13—C14—C15—N4	1.1 (4)

C1—O1—C5—C6	92.2 (2)	C12—O2—C16—C17	-97.0 (2)
C1—O1—C5—C10	-93.2 (2)	C12—O2—C16—C21	88.6 (2)
C10—C5—C6—C7	-0.3 (3)	C21—C16—C17—C18	-0.4 (3)
O1—C5—C6—C7	174.07 (18)	O2—C16—C17—C18	-174.54 (19)
C5—C6—C7—C8	0.1 (3)	C16—C17—C18—C19	0.0 (3)
C6—C7—C8—C9	0.4 (3)	C17—C18—C19—C20	-0.2 (4)
C7—C8—C9—C10	-0.7 (4)	C18—C19—C20—C21	0.7 (4)
C6—C5—C10—C9	0.0 (3)	C17—C16—C21—C20	0.9 (3)
O1—C5—C10—C9	-174.42 (19)	O2—C16—C21—C20	175.07 (19)
C6—C5—C10—C11	178.4 (2)	C17—C16—C21—C22	-178.4 (2)
O1—C5—C10—C11	4.0 (3)	O2—C16—C21—C22	-4.2 (3)
C8—C9—C10—C5	0.5 (3)	C19—C20—C21—C16	-1.1 (4)
C8—C9—C10—C11	-177.9 (2)	C19—C20—C21—C22	178.2 (2)
