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2-(*o*-Tolyloxy)pyrimidine

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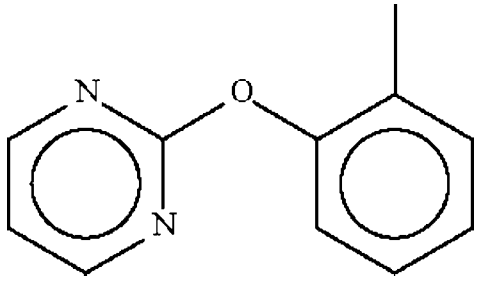
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.088; data-to-parameter ratio = 9.1.

The title compound, $C_{11}H_{10}N_2O$, 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-phenoxypyrimidine, see: Shah Bakhtiar *et al.* (2009).



Experimental

Crystal data

$C_{11}H_{10}N_2O$
M_r = 186.21
Orthorhombic, $Pca2_1$
a = 7.5197 (2) Å
b = 12.7997 (3) Å
c = 20.3238 (4) Å
V = 1956.16 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 153 K
0.35 × 0.25 × 0.15 mm

Data collection

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

Refinement

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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: *publCIF* (Westrip, 2009).

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

References

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supplementary materials

Acta Cryst. (2009). E**65**, o1880 [**doi:10.1107/S1600536809026609**]

2-(*o*-Tolyloxy)pyrimidine

N. Shah Bakhtiar, Z. Abdullah and S. W. Ng

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-chloropyridimidine (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.

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*(H) set to 1.2–1.5*U*(C).

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

Figures

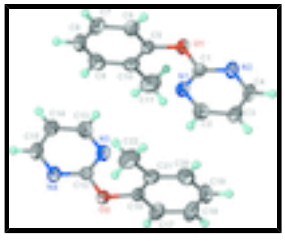


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{11}H_{10}N_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-(*o*-Tolyloxy)pyrimidine

Crystal data

$C_{11}H_{10}N_2O$	F_{000} = 784
M_r = 186.21	D_x = 1.265 Mg m^{-3}
Orthorhombic, *Pca*2$_1$	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 3906 reflections
a = 7.5197 (2) Å	θ = 2.6–27.9°
b = 12.7997 (3) Å	μ = 0.08 mm^{-1}
c = 20.3238 (4) Å	*T* = 153 K
V = 1956.16 (8) Å^3	Block, colorless
Z = 8	0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer	2030 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.028$
Monochromator: graphite	$\theta_{max} = 27.5°$
$T = 120$ K	$\theta_{min} = 1.6°$
ω scans	$h = -9 \rightarrow 9$
Absorption correction: None	$k = -16 \rightarrow 16$
12792 measured reflections	$l = -26 \rightarrow 26$
2317 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.088$	$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.3519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
2317 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
255 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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 (Å^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)

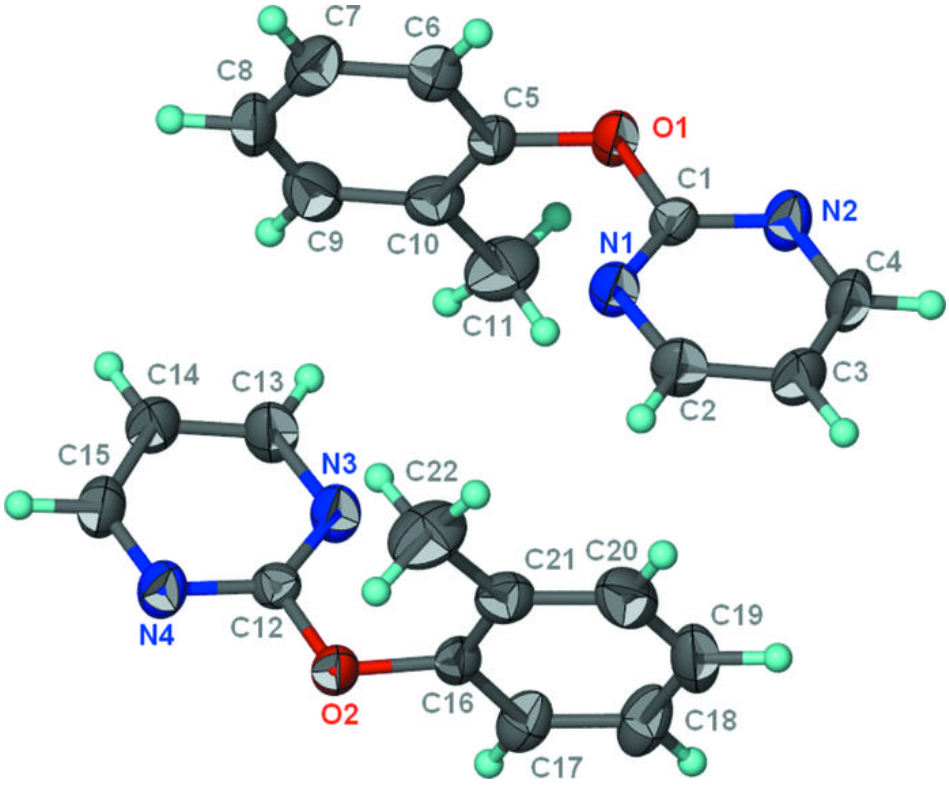
Geometric parameters (Å, °)

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)

Fig. 1


C7
C6
C8
C5
O1
C1
N2
C9
C10
N1
C4
C11
C3
C2
C14
C13
C15
N3
C22
C21
C20
C19
N4
C12
C16
O2
C18
C17