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2-(*p*-Tolyloxy)pyrimidine

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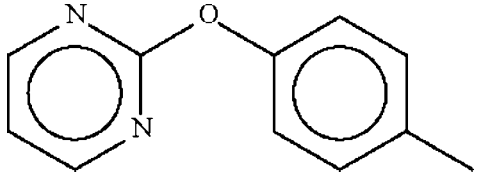
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.109; data-to-parameter ratio = 17.1.

In the title compound, $C_{11}H_{10}N_2O$, the aromatic rings make a dihedral angle of 76.3 (1)°. The C—O—C angle at the ether atom is widened to 117.79 (9)°.

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, *Pbca*
a = 11.2918 (2) Å
b = 7.2275 (1) Å
c = 23.3359 (5) Å
V = 1904.48 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 K
0.35 × 0.35 × 0.35 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
12308 measured reflections
2189 independent reflections
1789 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.109
S = 1.02
2189 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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: BT2996).

References

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supporting information

Acta Cryst. (2009). E**65**, o1859 [doi:10.1107/S1600536809026610]

2-(*p*-Tolyloxy)pyrimidine

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S1. Experimental

p-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 was extracted with chloroform. The chloroform solution was dried over sodium sulfate; slow evaporation led to the formation of colorless crystals.

S2. Refinement

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).

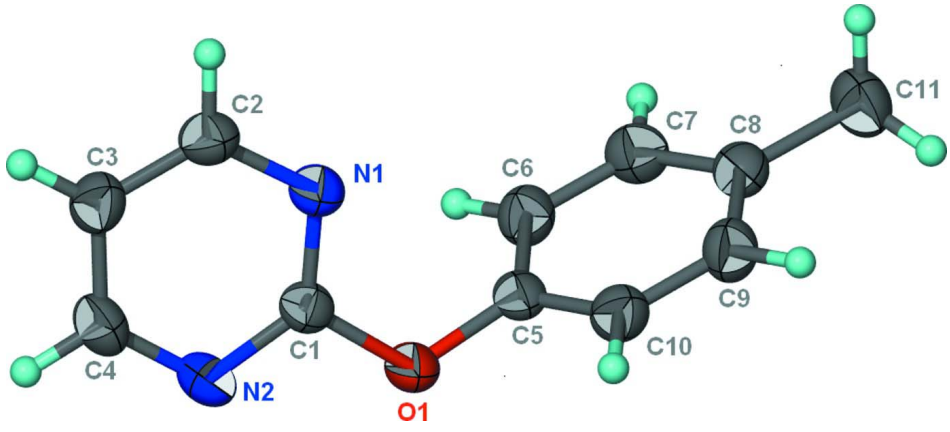

Figure 1

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

$C_{11}H_{10}N_2O$
M_r = 186.21
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 11.2918 (2) Å
b = 7.2275 (1) Å
c = 23.3359 (5) Å
V = 1904.48 (6) Å^3
Z = 8
F(000) = 784
D_x = 1.299 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3922 reflections
θ = 2.8–28.2°
μ = 0.09 mm^{-1}
T = 153 K
Irregular, colorless
0.35 × 0.35 × 0.35 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
12308 measured reflections
2189 independent reflections
1789 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -14 \rightarrow 13$
$k = -9 \rightarrow 9$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.109$
$S = 1.02$
2189 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.6197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.27705 (7)	0.18284 (13)	0.40394 (4)	0.0310 (2)
N1	0.38531 (9)	0.28051 (15)	0.48203 (4)	0.0294 (2)
N2	0.17358 (8)	0.27108 (15)	0.48092 (4)	0.0303 (3)
C1	0.28062 (9)	0.24949 (16)	0.45862 (5)	0.0253 (3)
C2	0.38117 (11)	0.34394 (19)	0.53603 (5)	0.0330 (3)
H2	0.4534	0.3703	0.5552	0.040*
C3	0.27601 (11)	0.37220 (19)	0.56462 (5)	0.0334 (3)
H3	0.2743	0.4166	0.6029	0.040*
C4	0.17305 (11)	0.33291 (18)	0.53495 (5)	0.0332 (3)
H4	0.0992	0.3505	0.5536	0.040*
C5	0.38237 (10)	0.18523 (17)	0.37209 (5)	0.0272 (3)
C6	0.42753 (11)	0.35123 (18)	0.35269 (5)	0.0319 (3)
H6	0.3916	0.4650	0.3633	0.038*
C7	0.52621 (11)	0.34878 (18)	0.31740 (5)	0.0335 (3)
H7	0.5580	0.4625	0.3040	0.040*
C8	0.57990 (11)	0.18345 (18)	0.30110 (5)	0.0305 (3)
C9	0.53213 (11)	0.01971 (18)	0.32187 (5)	0.0339 (3)
H9	0.5677	−0.0946	0.3115	0.041*
C10	0.43334 (11)	0.01911 (18)	0.35755 (5)	0.0318 (3)
H10	0.4018	−0.0940	0.3716	0.038*
C11	0.68626 (13)	0.1829 (2)	0.26196 (6)	0.0416 (3)
H11A	0.7585	0.1985	0.2847	0.062*
H11B	0.6796	0.2848	0.2344	0.062*
H11C	0.6898	0.0650	0.2413	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0222 (4)	0.0426 (5)	0.0281 (4)	−0.0027 (4)	−0.0013 (3)	−0.0065 (4)
N1	0.0229 (5)	0.0361 (6)	0.0291 (5)	−0.0004 (4)	−0.0016 (4)	−0.0035 (4)
N2	0.0215 (5)	0.0360 (6)	0.0335 (5)	−0.0015 (4)	0.0020 (4)	0.0026 (4)
C1	0.0239 (6)	0.0248 (6)	0.0271 (6)	0.0001 (4)	−0.0007 (4)	0.0011 (4)
C2	0.0296 (6)	0.0397 (7)	0.0298 (6)	−0.0048 (5)	−0.0025 (5)	−0.0034 (5)
C3	0.0369 (7)	0.0353 (7)	0.0279 (6)	−0.0040 (5)	0.0048 (5)	−0.0026 (5)
C4	0.0281 (6)	0.0374 (7)	0.0343 (6)	−0.0006 (5)	0.0085 (5)	0.0017 (5)
C5	0.0219 (5)	0.0369 (7)	0.0227 (5)	−0.0008 (5)	−0.0028 (4)	−0.0028 (5)
C6	0.0326 (6)	0.0305 (6)	0.0327 (6)	0.0034 (5)	−0.0003 (5)	−0.0022 (5)
C7	0.0354 (7)	0.0317 (6)	0.0333 (6)	−0.0033 (5)	0.0002 (5)	0.0032 (5)
C8	0.0287 (6)	0.0371 (7)	0.0256 (6)	−0.0010 (5)	−0.0008 (5)	−0.0018 (5)
C9	0.0356 (7)	0.0309 (6)	0.0352 (7)	0.0024 (5)	0.0045 (5)	−0.0038 (5)
C10	0.0336 (6)	0.0305 (6)	0.0313 (6)	−0.0039 (5)	0.0017 (5)	−0.0016 (5)
C11	0.0368 (7)	0.0461 (8)	0.0420 (8)	−0.0015 (6)	0.0096 (6)	−0.0012 (6)

Geometric parameters (Å, º)

O1—C1	1.3644 (14)	C6—C7	1.3856 (18)
O1—C5	1.4026 (14)	C6—H6	0.9500
N1—C1	1.3215 (14)	C7—C8	1.3928 (18)
N1—C2	1.3419 (16)	C7—H7	0.9500
N2—C1	1.3252 (15)	C8—C9	1.3880 (18)
N2—C4	1.3376 (17)	C8—C11	1.5090 (17)
C2—C3	1.3773 (18)	C9—C10	1.3919 (17)
C2—H2	0.9500	C9—H9	0.9500
C3—C4	1.3826 (18)	C10—H10	0.9500
C3—H3	0.9500	C11—H11A	0.9800
C4—H4	0.9500	C11—H11B	0.9800
C5—C10	1.3740 (17)	C11—H11C	0.9800
C5—C6	1.3801 (17)		
C1—O1—C5	117.79 (9)	C7—C6—H6	120.6
C1—N1—C2	114.53 (10)	C6—C7—C8	121.55 (12)
C1—N2—C4	114.44 (10)	C6—C7—H7	119.2
N1—C1—N2	129.31 (11)	C8—C7—H7	119.2
N1—C1—O1	118.23 (10)	C9—C8—C7	117.84 (11)
N2—C1—O1	112.45 (10)	C9—C8—C11	121.23 (12)
N1—C2—C3	122.38 (11)	C7—C8—C11	120.94 (12)
N1—C2—H2	118.8	C8—C9—C10	121.53 (12)
C3—C2—H2	118.8	C8—C9—H9	119.2
C2—C3—C4	116.87 (12)	C10—C9—H9	119.2
C2—C3—H3	121.6	C5—C10—C9	118.73 (12)
C4—C3—H3	121.6	C5—C10—H10	120.6
N2—C4—C3	122.47 (11)	C9—C10—H10	120.6
N2—C4—H4	118.8	C8—C11—H11A	109.5

C3—C4—H4	118.8	C8—C11—H11B	109.5
C10—C5—C6	121.59 (11)	H11A—C11—H11B	109.5
C10—C5—O1	118.38 (11)	C8—C11—H11C	109.5
C6—C5—O1	119.86 (11)	H11A—C11—H11C	109.5
C5—C6—C7	118.75 (12)	H11B—C11—H11C	109.5
C5—C6—H6	120.6		

C2—N1—C1—N2	−0.4 (2)	C1—O1—C5—C6	−71.51 (14)
C2—N1—C1—O1	−179.29 (11)	C10—C5—C6—C7	0.44 (18)
C4—N2—C1—N1	−0.13 (19)	O1—C5—C6—C7	−174.79 (10)
C4—N2—C1—O1	178.78 (10)	C5—C6—C7—C8	0.27 (19)
C5—O1—C1—N1	−12.16 (16)	C6—C7—C8—C9	−0.69 (19)
C5—O1—C1—N2	168.79 (10)	C6—C7—C8—C11	179.10 (12)
C1—N1—C2—C3	0.64 (19)	C7—C8—C9—C10	0.42 (19)
N1—C2—C3—C4	−0.3 (2)	C11—C8—C9—C10	−179.37 (12)
C1—N2—C4—C3	0.51 (18)	C6—C5—C10—C9	−0.70 (18)
C2—C3—C4—N2	−0.3 (2)	O1—C5—C10—C9	174.60 (10)
C1—O1—C5—C10	113.10 (12)	C8—C9—C10—C5	0.26 (19)