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4-Amino-2-phenoxypyrimidine

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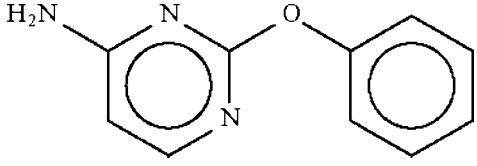
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.163; data-to-parameter ratio = 16.0.

In the title compound, $C_{10}H_9N_3O$, the organic rings linked to the ether O atom make a dihedral angle of 76.8 (1)° and the C—O—C angle is widened to 119.07 (15)°. In the crystal, adjacent molecules are connected by an N—H···N hydrogen bond, generating a chain running parallel to the b axis. The crystal is a non-merohedral twin with a ratio of twin components of 0.508 (3):0.492 (3).

Related literature

For 2-phenoxypyrimidine, see: Shah Bakhtiar *et al.* (2009). For the procedure to cope with twinned diffraction data, see: Spek (2003).



Experimental

Crystal data

$C_{10}H_9N_3O$
M_r = 187.20
Monoclinic, $P2_1/n$
a = 8.8443 (3) Å
b = 12.1214 (3) Å
c = 9.0415 (2) Å
β = 96.751 (2)°
V = 962.58 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 K
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
6375 measured reflections
2178 independent reflections
1694 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.163
S = 1.10
2178 reflections
136 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1···N1^{i}	0.88 (1)	2.12 (1)	2.992 (2)	173 (2)

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

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: BT2994).

References

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supplementary materials

Acta Cryst. (2009). E**65**, o1858 [**doi:10.1107/S1600536809026580**]

4-Amino-2-phenoxypyrimidine

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

Experimental

Phenol (1.88 g, 20 mmol) and sodium hydroxide (0.80 g, 20 mmol) were dissolved in water (50 ml) and to the solution was added 4-amino-2-chloropyridimidine (2.60 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.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). The H atoms bonded to N were freely refined.

The crystal is a non-merohedral twin; the twin law as given by *PLATON* is (Spek, 2003) (-1 0 0, 0 - 1 0, 0.240 0 1); the refinement gave a ratio of twin components of 0.508 (3)/0.492 (3).

Figures

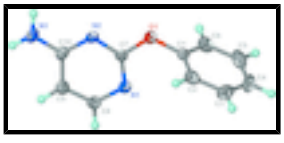

Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{10}H_9N_3O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-Amino-2-phenoxypyrimidine

Crystal data

$C_{10}H_9N_3O$	F_{000} = 392
M_r = 187.20	D_x = 1.292 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2238 reflections
a = 8.8443 (3) Å	θ = 2.3–27.9º
b = 12.1214 (3) Å	μ = 0.09 mm^{-1}
c = 9.0415 (2) Å	T = 120 K
β = 96.751 (2)º	Block, colorless
V = 962.58 (5) Å^3	0.40 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEX	1694 reflections with $I > 2\sigma(I)$

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 120 K

ω scans

Absorption correction: None

6375 measured reflections

2178 independent reflections

R_{int} = 0.028

θ_{max} = 27.5º

θ_{min} = 2.8º

h = −10→11

k = −15→15

l = −10→11

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.055

$wR(F^2)$ = 0.163

S = 1.10

2178 reflections

136 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0791P)^2 + 0.3378P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.43 e Å^{-3}

$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.2422 (2)	0.48867 (12)	−0.00659 (16)	0.0317 (4)
N1	0.2790 (2)	0.36872 (13)	0.19209 (18)	0.0235 (4)
N2	0.2591 (2)	0.56448 (13)	0.21860 (17)	0.0213 (4)
N3	0.2755 (3)	0.64646 (15)	0.4479 (2)	0.0348 (5)
H1	0.252 (3)	0.7092 (13)	0.402 (2)	0.030 (7)*
H2	0.284 (3)	0.641 (2)	0.5458 (11)	0.037 (7)*
C1	0.2551 (3)	0.39941 (16)	−0.1029 (2)	0.0220 (5)
C2	0.3964 (3)	0.35937 (18)	−0.1237 (2)	0.0264 (5)
H2A	0.4857	0.3889	−0.0693	0.032*
C3	0.4063 (3)	0.27495 (19)	−0.2257 (2)	0.0339 (6)
H3	0.5030	0.2460	−0.2410	0.041*
C4	0.2763 (4)	0.23278 (18)	−0.3052 (2)	0.0369 (7)
H4	0.2836	0.1744	−0.3741	0.044*
C5	0.1354 (3)	0.2756 (2)	−0.2843 (2)	0.0374 (6)
H5	0.0461	0.2475	−0.3403	0.045*
C6	0.1240 (3)	0.35942 (19)	−0.1819 (2)	0.0307 (5)
H6	0.0274	0.3887	−0.1665	0.037*
C7	0.2617 (2)	0.47102 (16)	0.1428 (2)	0.0197 (4)
C8	0.2997 (3)	0.36125 (17)	0.3429 (2)	0.0283 (5)
H8	0.3133	0.2900	0.3862	0.034*

C9	0.3022 (3)	0.44951 (17)	0.4354 (2)	0.0296 (5)
H9	0.3190	0.4413	0.5405	0.036*
C10	0.2785 (3)	0.55438 (16)	0.3677 (2)	0.0236 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0606 (12)	0.0159 (7)	0.0178 (7)	0.0050 (7)	0.0018 (7)	0.0013 (5)
N1	0.0341 (11)	0.0165 (8)	0.0197 (8)	0.0014 (7)	0.0032 (7)	0.0007 (6)
N2	0.0281 (10)	0.0149 (8)	0.0212 (8)	0.0028 (7)	0.0038 (7)	0.0003 (6)
N3	0.0665 (16)	0.0182 (9)	0.0204 (9)	0.0070 (9)	0.0083 (9)	−0.0008 (7)
C1	0.0351 (13)	0.0156 (9)	0.0151 (9)	0.0006 (8)	0.0018 (8)	0.0031 (7)
C2	0.0301 (12)	0.0255 (10)	0.0229 (10)	−0.0038 (9)	0.0005 (9)	0.0044 (8)
C3	0.0476 (15)	0.0264 (11)	0.0310 (11)	0.0084 (11)	0.0186 (11)	0.0062 (9)
C4	0.073 (2)	0.0193 (10)	0.0198 (10)	−0.0061 (12)	0.0127 (11)	−0.0026 (8)
C5	0.0511 (17)	0.0348 (12)	0.0238 (11)	−0.0161 (12)	−0.0058 (11)	0.0001 (9)
C6	0.0311 (13)	0.0319 (12)	0.0284 (11)	0.0006 (10)	0.0013 (10)	0.0036 (9)
C7	0.0217 (11)	0.0186 (9)	0.0185 (9)	0.0015 (8)	0.0012 (8)	0.0019 (7)
C8	0.0455 (14)	0.0174 (9)	0.0221 (10)	0.0044 (9)	0.0046 (9)	0.0046 (7)
C9	0.0482 (15)	0.0216 (10)	0.0194 (9)	0.0028 (10)	0.0057 (9)	0.0027 (7)
C10	0.0312 (12)	0.0181 (9)	0.0223 (9)	0.0008 (8)	0.0062 (9)	−0.0007 (7)

Geometric parameters (Å, °)

O1—C7	1.359 (2)	C2—H2A	0.9500
O1—C1	1.402 (2)	C3—C4	1.380 (4)
N1—C7	1.320 (2)	C3—H3	0.9500
N1—C8	1.357 (3)	C4—C5	1.384 (4)
N2—C7	1.326 (2)	C4—H4	0.9500
N2—C10	1.344 (2)	C5—C6	1.386 (3)
N3—C10	1.333 (3)	C5—H5	0.9500
N3—H1	0.880 (10)	C6—H6	0.9500
N3—H2	0.882 (10)	C8—C9	1.356 (3)
C1—C2	1.375 (3)	C8—H8	0.9500
C1—C6	1.376 (3)	C9—C10	1.416 (3)
C2—C3	1.387 (3)	C9—H9	0.9500
C7—O1—C1	119.07 (15)	C4—C5—C6	120.2 (2)
C7—N1—C8	113.46 (17)	C4—C5—H5	119.9
C7—N2—C10	115.63 (16)	C6—C5—H5	119.9
C10—N3—H1	119.1 (16)	C1—C6—C5	118.8 (2)
C10—N3—H2	118.5 (18)	C1—C6—H6	120.6
H1—N3—H2	122 (2)	C5—C6—H6	120.6
C2—C1—C6	121.9 (2)	N1—C7—N2	129.54 (18)
C2—C1—O1	120.0 (2)	N1—C7—O1	118.65 (17)
C6—C1—O1	118.0 (2)	N2—C7—O1	111.80 (16)
C1—C2—C3	118.7 (2)	C9—C8—N1	123.86 (18)
C1—C2—H2A	120.6	C9—C8—H8	118.1
C3—C2—H2A	120.6	N1—C8—H8	118.1

C4—C3—C2	120.4 (2)	C8—C9—C10	116.79 (18)
C4—C3—H3	119.8	C8—C9—H9	121.6
C2—C3—H3	119.8	C10—C9—H9	121.6
C3—C4—C5	119.9 (2)	N3—C10—N2	117.46 (18)
C3—C4—H4	120.0	N3—C10—C9	121.85 (18)
C5—C4—H4	120.0	N2—C10—C9	120.69 (18)
C7—O1—C1—C2	−76.8 (2)	C8—N1—C7—O1	179.1 (2)
C7—O1—C1—C6	107.6 (2)	C10—N2—C7—N1	0.8 (3)
C6—C1—C2—C3	−1.1 (3)	C10—N2—C7—O1	−179.63 (19)
O1—C1—C2—C3	−176.53 (17)	C1—O1—C7—N1	−5.8 (3)
C1—C2—C3—C4	0.4 (3)	C1—O1—C7—N2	174.56 (18)
C2—C3—C4—C5	0.7 (3)	C7—N1—C8—C9	0.2 (4)
C3—C4—C5—C6	−1.2 (3)	N1—C8—C9—C10	1.3 (4)
C2—C1—C6—C5	0.6 (3)	C7—N2—C10—N3	−179.5 (2)
O1—C1—C6—C5	176.15 (18)	C7—N2—C10—C9	0.9 (3)
C4—C5—C6—C1	0.5 (3)	C8—C9—C10—N3	178.6 (2)
C8—N1—C7—N2	−1.3 (3)	C8—C9—C10—N2	−1.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1···N1^{i}	0.88 (1)	2.12 (1)	2.992 (2)	173 (2)

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+1/2.

Fig. 1