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Quinoxalin-2-yl *m*-tolyl ether

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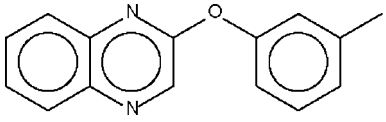
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.112; data-to-parameter ratio = 16.5.

The dihedral angle between the two aromatic ring systems in the title compound, $C_{15}H_{12}N_2O$, is 79.4 (1)°. The angle at the O atom is widened to 116.93 (9)°.

Related literature

The title compound exhibits fluorescence; see: Abdullah (2005); Kawai *et al.* (2001); Mohd Salleh *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{12}N_2O$
M_r = 236.27
Monoclinic, $C2/c$
a = 18.5958 (5) Å
b = 7.0710 (1) Å
c = 19.4821 (5) Å
β = 112.487 (1)°
V = 2366.94 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.40 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
8036 measured reflections
2708 independent reflections
2179 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.04
2708 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2770).

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supplementary materials

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Quinoxalin-2-yl *m*-tolyl ether

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Comment

(type here to add)

Experimental

m-Cresol (0.54 g, 5 mmol) was dissolved in a small volume of water containing potassium hydroxide (0.20 g, 5 mmol). The mixture was heated to remove the water to give a brown compound. The compound and 2-chloroquinoxaline (0.82, g, 5 mmol) were heated in THF (15 ml) for 8 h. The mixture was in 1 N sodium hydroxide; the aqueous solution was extracted with dichloromethane. The organic phase was dried over sodium sulfate. Evaporation of the solvent gave a yellow product, which was was washed with chloroform to remove impurities. Crystals were obtained upon recrystallization from an ethyl acetate/hexane mixture.

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) fixed at 1.2–1.5*U*(C).

Figures

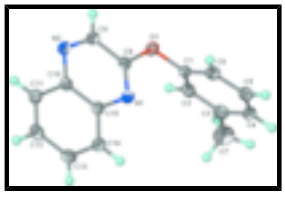

Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of $C_{15}H_{12}N_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Quinoxalin-2-yl *m*-tolyl ether

Crystal data

$C_{15}H_{12}N_2O$	F_{000} = 992
M_r = 236.27	D_x = 1.326 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 756 reflections
a = 18.5958 (5) Å	θ = 2.7–24.6º
b = 7.0710 (1) Å	μ = 0.09 mm^{-1}
c = 19.4821 (5) Å	*T* = 100 (2) K
β = 112.487 (1)º	Block, colorless

V = 2366.94 (9) Å^3
Z = 8

0.40 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 100(2) K
ω scans
Absorption correction: None
8036 measured reflections
2708 independent reflections

2179 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.5º
θ_{min} = 2.3º
h = −24→24
k = −9→9
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.04
2708 reflections
164 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
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 1.0233P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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	0.67552 (5)	0.84219 (13)	0.54655 (5)	0.0215 (2)
N1	0.58519 (6)	0.74119 (14)	0.59395 (5)	0.0174 (2)
N2	0.47213 (6)	0.77607 (15)	0.44719 (6)	0.0200 (2)
C1	0.73297 (7)	0.83475 (17)	0.61927 (7)	0.0179 (3)
C2	0.78445 (7)	0.68518 (17)	0.63734 (7)	0.0202 (3)
H2	0.7802	0.5894	0.6018	0.024*
C3	0.84288 (7)	0.67583 (18)	0.70839 (7)	0.0223 (3)
C4	0.84907 (7)	0.82240 (19)	0.75792 (7)	0.0215 (3)
H4	0.8893	0.8193	0.8060	0.026*
C5	0.79743 (7)	0.97296 (18)	0.73822 (7)	0.0220 (3)
H5	0.8027	1.0723	0.7727	0.026*
C6	0.73806 (7)	0.97912 (17)	0.66841 (7)	0.0206 (3)
H6	0.7018	1.0804	0.6548	0.025*
C7	0.89521 (8)	0.5050 (2)	0.73175 (9)	0.0364 (4)
H7A	0.9393	0.5328	0.7781	0.055*
H7B	0.9145	0.4736	0.6929	0.055*

H7C	0.8658	0.3977	0.7395	0.055*
C8	0.60151 (7)	0.79686 (16)	0.53826 (7)	0.0174 (3)
C9	0.54531 (7)	0.81523 (17)	0.46401 (7)	0.0192 (3)
H9	0.5618	0.8570	0.4260	0.023*
C10	0.45167 (7)	0.71606 (16)	0.50459 (7)	0.0176 (3)
C11	0.37355 (7)	0.66926 (17)	0.48997 (7)	0.0218 (3)
H11	0.3356	0.6792	0.4408	0.026*
C12	0.35219 (7)	0.60961 (18)	0.54625 (7)	0.0230 (3)
H12	0.2994	0.5791	0.5362	0.028*
C13	0.40826 (7)	0.59334 (17)	0.61903 (7)	0.0219 (3)
H13	0.3930	0.5512	0.6577	0.026*
C14	0.48469 (7)	0.63759 (17)	0.63472 (7)	0.0194 (3)
H14	0.5219	0.6266	0.6841	0.023*
C15	0.50814 (7)	0.69927 (16)	0.57774 (7)	0.0163 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0167 (4)	0.0313 (5)	0.0162 (4)	−0.0030 (4)	0.0059 (3)	0.0016 (4)
N1	0.0173 (5)	0.0183 (5)	0.0161 (5)	0.0006 (4)	0.0057 (4)	0.0004 (4)
N2	0.0221 (6)	0.0191 (5)	0.0168 (5)	−0.0012 (4)	0.0051 (4)	0.0003 (4)
C1	0.0150 (6)	0.0236 (6)	0.0156 (6)	−0.0040 (5)	0.0063 (5)	0.0018 (5)
C2	0.0197 (6)	0.0207 (6)	0.0228 (6)	−0.0035 (5)	0.0108 (5)	−0.0027 (5)
C3	0.0173 (6)	0.0252 (6)	0.0266 (7)	0.0009 (5)	0.0106 (5)	0.0046 (5)
C4	0.0160 (6)	0.0301 (7)	0.0176 (6)	−0.0044 (5)	0.0055 (5)	0.0027 (5)
C5	0.0240 (7)	0.0248 (6)	0.0201 (6)	−0.0051 (5)	0.0116 (5)	−0.0028 (5)
C6	0.0203 (6)	0.0213 (6)	0.0223 (6)	0.0011 (5)	0.0104 (5)	0.0017 (5)
C7	0.0294 (8)	0.0366 (8)	0.0422 (9)	0.0122 (6)	0.0127 (7)	0.0077 (7)
C8	0.0167 (6)	0.0168 (6)	0.0190 (6)	0.0001 (4)	0.0071 (5)	−0.0010 (5)
C9	0.0220 (7)	0.0197 (6)	0.0161 (6)	−0.0009 (5)	0.0076 (5)	0.0005 (5)
C10	0.0194 (6)	0.0141 (5)	0.0186 (6)	0.0004 (4)	0.0065 (5)	−0.0001 (5)
C11	0.0180 (6)	0.0209 (6)	0.0218 (6)	−0.0007 (5)	0.0023 (5)	0.0011 (5)
C12	0.0178 (6)	0.0227 (6)	0.0291 (7)	−0.0027 (5)	0.0097 (5)	−0.0005 (5)
C13	0.0251 (7)	0.0200 (6)	0.0237 (6)	−0.0011 (5)	0.0128 (5)	0.0004 (5)
C14	0.0213 (6)	0.0190 (6)	0.0180 (6)	0.0003 (5)	0.0074 (5)	0.0003 (5)
C15	0.0178 (6)	0.0133 (5)	0.0172 (6)	0.0010 (4)	0.0060 (5)	−0.0016 (4)

Geometric parameters (Å, °)

O1—C8	1.3612 (14)	C6—H6	0.9500
O1—C1	1.4119 (14)	C7—H7A	0.9800
N1—C8	1.2947 (16)	C7—H7B	0.9800
N1—C15	1.3764 (15)	C7—H7C	0.9800
N2—C9	1.3018 (15)	C8—C9	1.4302 (17)
N2—C10	1.3787 (16)	C9—H9	0.9500
C1—C6	1.3778 (17)	C10—C11	1.4087 (17)
C1—C2	1.3787 (17)	C10—C15	1.4153 (16)
C2—C3	1.3967 (17)	C11—C12	1.3678 (18)
C2—H2	0.9500	C11—H11	0.9500

C3—C4	1.3905 (19)	C12—C13	1.4071 (18)
C3—C7	1.5080 (18)	C12—H12	0.9500
C4—C5	1.3859 (18)	C13—C14	1.3707 (17)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.3863 (17)	C14—C15	1.4082 (17)
C5—H5	0.9500	C14—H14	0.9500
C8—O1—C1	116.93 (9)	H7B—C7—H7C	109.5
C8—N1—C15	115.49 (10)	N1—C8—O1	121.51 (11)
C9—N2—C10	116.58 (10)	N1—C8—C9	124.08 (11)
C6—C1—C2	122.30 (11)	O1—C8—C9	114.41 (10)
C6—C1—O1	119.61 (11)	N2—C9—C8	121.63 (11)
C2—C1—O1	118.02 (11)	N2—C9—H9	119.2
C1—C2—C3	119.36 (11)	C8—C9—H9	119.2
C1—C2—H2	120.3	N2—C10—C11	119.44 (11)
C3—C2—H2	120.3	N2—C10—C15	120.93 (11)
C4—C3—C2	118.62 (11)	C11—C10—C15	119.63 (11)
C4—C3—C7	121.00 (12)	C12—C11—C10	120.23 (12)
C2—C3—C7	120.30 (12)	C12—C11—H11	119.9
C5—C4—C3	121.04 (11)	C10—C11—H11	119.9
C5—C4—H4	119.5	C11—C12—C13	120.17 (12)
C3—C4—H4	119.5	C11—C12—H12	119.9
C6—C5—C4	120.22 (12)	C13—C12—H12	119.9
C6—C5—H5	119.9	C14—C13—C12	120.76 (12)
C4—C5—H5	119.9	C14—C13—H13	119.6
C1—C6—C5	118.40 (12)	C12—C13—H13	119.6
C1—C6—H6	120.8	C13—C14—C15	120.15 (11)
C5—C6—H6	120.8	C13—C14—H14	119.9
C3—C7—H7A	109.5	C15—C14—H14	119.9
C3—C7—H7B	109.5	N1—C15—C14	119.66 (11)
H7A—C7—H7B	109.5	N1—C15—C10	121.29 (11)
C3—C7—H7C	109.5	C14—C15—C10	119.05 (11)
H7A—C7—H7C	109.5		
C8—O1—C1—C6	−77.38 (14)	N1—C8—C9—N2	−0.01 (19)
C8—O1—C1—C2	105.36 (13)	O1—C8—C9—N2	179.64 (11)
C6—C1—C2—C3	1.58 (18)	C9—N2—C10—C11	−179.26 (11)
O1—C1—C2—C3	178.76 (10)	C9—N2—C10—C15	0.17 (17)
C1—C2—C3—C4	−2.44 (18)	N2—C10—C11—C12	−179.95 (11)
C1—C2—C3—C7	174.40 (12)	C15—C10—C11—C12	0.61 (18)
C2—C3—C4—C5	1.48 (18)	C10—C11—C12—C13	−0.45 (19)
C7—C3—C4—C5	−175.34 (12)	C11—C12—C13—C14	0.31 (19)
C3—C4—C5—C6	0.41 (18)	C12—C13—C14—C15	−0.33 (19)
C2—C1—C6—C5	0.31 (18)	C8—N1—C15—C14	−179.98 (11)
O1—C1—C6—C5	−176.82 (10)	C8—N1—C15—C10	0.31 (16)
C4—C5—C6—C1	−1.31 (18)	C13—C14—C15—N1	−179.24 (11)
C15—N1—C8—O1	−179.77 (10)	C13—C14—C15—C10	0.48 (18)
C15—N1—C8—C9	−0.15 (17)	N2—C10—C15—N1	−0.33 (17)
C1—O1—C8—N1	−3.05 (16)	C11—C10—C15—N1	179.09 (11)
C1—O1—C8—C9	177.29 (10)	N2—C10—C15—C14	179.95 (11)

C10—N2—C9—C8	0.00 (17)	C11—C10—C15—C14	−0.62 (17)

Fig. 1