Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Quinoxalin-2-yl *m*-tolyl ether

Nor Duha Hassan, Hairul Anuar Tajuddin, Zanariah Abdullah and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

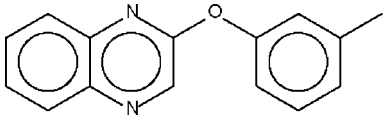
Received 12 August 2008; accepted 19 August 2008

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).

We thank the University of Malaya for supporting this study (grant No. 358/2008 A).

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

References

Abdullah, Z. (2005). *Int. J. Chem. Sci.* **3**, 9–15.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kawai, M., Lee, M. J., Evans, K. O. & Norlund, T. (2001). *J. Fluoresc.* **11**, 23–32.
Mohd Salleh, N., Ling, L. P., Abdullah, Z. M. A. A. & Aiyub, Z. (2007). *Malays. J. Anal. Sci.* **11**, 229–236.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supporting information

Acta Cryst. (2008). E**64**, o1822 [doi:10.1107/S1600536808026822]

Quinoxalin-2-yl *m*-tolyl ether

Nor Duha Hassan, Hairul Anuar Tajuddin, Zanariah Abdullah and Seik Weng Ng

S1. 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.

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*(H) fixed at 1.2–1.5*U*(C).

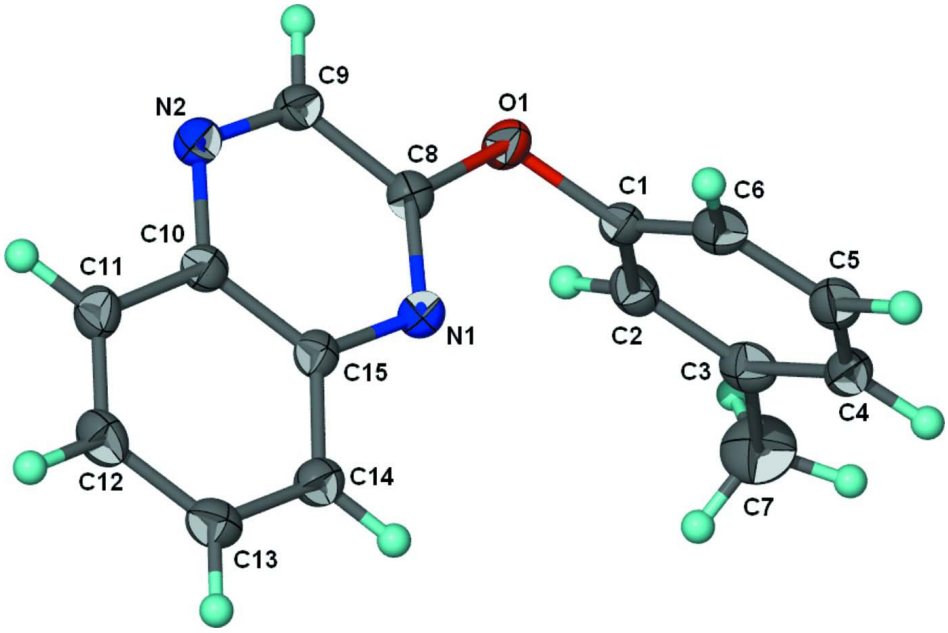


Figure 1

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

$C_{15}H_{12}N_2O$
$M_r = 236.27$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 18.5958$ (5) Å
$b = 7.0710$ (1) Å
$c = 19.4821$ (5) Å
$\beta = 112.487$ (1)°
$V = 2366.94$ (9) Å^3
$Z = 8$
$F(000) = 992$
$D_x = 1.326$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 756 reflections
$\theta = 2.7$–$24.6°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Block, colorless
0.40 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
8036 measured reflections
2708 independent reflections
2179 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -24 \rightarrow 24$
$k = -9 \rightarrow 9$
$l = -25 \rightarrow 25$

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
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
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 1.0233P]$ 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}

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 (Å²)

	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, º)

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)