Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Quinoxalin-2-yl *p*-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

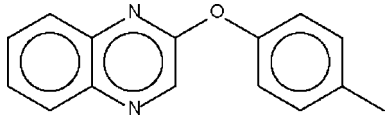
Received 12 August 2008; accepted 19 August 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.100; data-to-parameter ratio = 12.4.

The dihedral angle between the two aromatic ring systems in the title compound, $C_{15}H_{12}N_2O$, is 42.6 (1)°. The angle at the O atom is widened to 117.7 (1)°.

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
Triclinic, $P\overline{1}$
a = 5.2655 (1) Å
b = 9.1713 (2) Å
c = 12.8112 (2) Å
α = 74.660 (1)°
β = 81.163 (1)°
γ = 89.095 (1)°
V = 589.35 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.25 × 0.25 × 0.25 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
2828 measured reflections
2030 independent reflections
1764 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
S = 0.99
2030 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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: BT2771).

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**, o1823 [doi:10.1107/S1600536808026834]

Quinoxalin-2-yl *p*-tolyl ether

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

S1. Experimental

p-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).

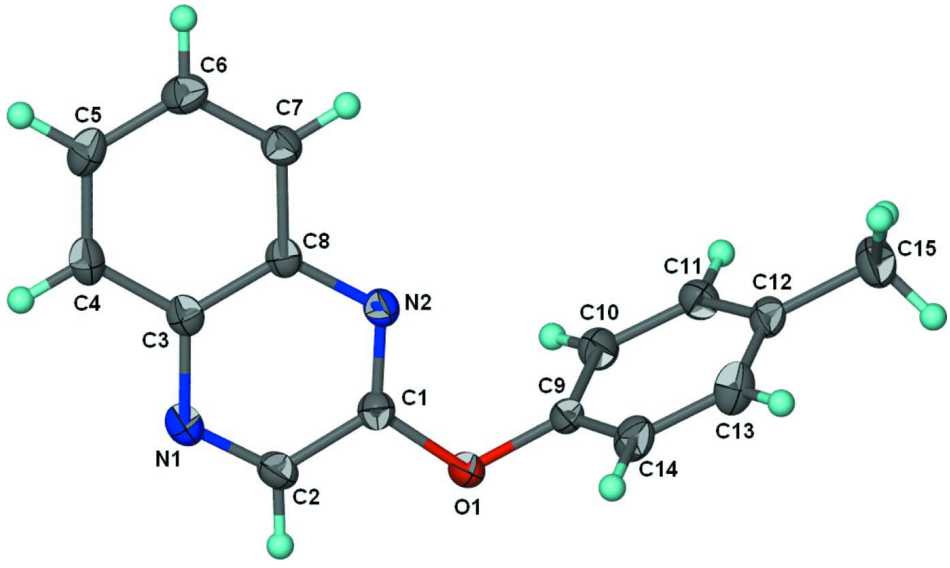


Figure 1

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

Quinoxalin-2-yl *p*-tolyl ether

Crystal data

$C_{15}H_{12}N_2O$
$M_r = 236.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.2655$ (1) Å
$b = 9.1713$ (2) Å
$c = 12.8112$ (2) Å
$\alpha = 74.660$ (1)°
$\beta = 81.163$ (1)°
$\gamma = 89.095$ (1)°
$V = 589.35$ (2) Å^3
$Z = 2$
$F(000) = 248$
$D_x = 1.331$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2687 reflections
$\theta = 2.3$–$28.3°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Irregular block, colorless
0.25 × 0.25 × 0.25 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
2828 measured reflections
2030 independent reflections
1764 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -6 \rightarrow 6$
$k = -7 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.099$
$S = 0.99$
2030 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
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.1439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.26514 (16)	1.02668 (10)	0.14690 (7)	0.0230 (2)
N1	1.07057 (19)	0.73809 (12)	0.03457 (8)	0.0218 (3)
N2	0.91228 (18)	0.86256 (11)	0.21386 (8)	0.0189 (2)
C1	1.1133 (2)	0.91123 (13)	0.14121 (10)	0.0188 (3)
C2	1.1953 (2)	0.84960 (14)	0.05056 (10)	0.0216 (3)
H2	1.3450	0.8912	0.0006	0.026*
C3	0.8547 (2)	0.68201 (13)	0.10938 (10)	0.0192 (3)
C4	0.7105 (2)	0.56145 (14)	0.09688 (10)	0.0232 (3)
H4	0.7628	0.5188	0.0373	0.028*
C5	0.4948 (2)	0.50557 (14)	0.17061 (11)	0.0245 (3)
H5	0.3980	0.4242	0.1619	0.029*
C6	0.4161 (2)	0.56796 (14)	0.25901 (10)	0.0237 (3)
H6	0.2654	0.5290	0.3093	0.028*

C7	0.5546 (2)	0.68464 (14)	0.27340 (10)	0.0217 (3)
H7	0.5005	0.7252	0.3339	0.026*
C8	0.7766 (2)	0.74447 (13)	0.19880 (10)	0.0181 (3)
C9	1.1976 (2)	1.09150 (13)	0.23540 (10)	0.0199 (3)
C10	0.9936 (2)	1.18709 (14)	0.23647 (10)	0.0232 (3)
H10	0.8934	1.2083	0.1788	0.028*
C11	0.9373 (2)	1.25183 (14)	0.32362 (10)	0.0229 (3)
H11	0.7965	1.3177	0.3252	0.028*
C12	1.0819 (2)	1.22244 (13)	0.40840 (10)	0.0212 (3)
C13	1.2913 (2)	1.12925 (14)	0.40226 (11)	0.0259 (3)
H13	1.3958	1.1102	0.4584	0.031*
C14	1.3511 (2)	1.06353 (14)	0.31607 (11)	0.0241 (3)
H14	1.4953	1.0004	0.3127	0.029*
C15	1.0175 (3)	1.29050 (15)	0.50378 (10)	0.0292 (3)
H15A	0.8638	1.3514	0.4951	0.044*
H15B	1.1620	1.3549	0.5063	0.044*
H15C	0.9849	1.2095	0.5720	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0225 (4)	0.0229 (5)	0.0243 (5)	−0.0055 (4)	0.0043 (4)	−0.0114 (4)
N1	0.0235 (5)	0.0231 (6)	0.0198 (5)	0.0028 (4)	−0.0031 (4)	−0.0081 (4)
N2	0.0203 (5)	0.0176 (5)	0.0190 (5)	0.0008 (4)	−0.0021 (4)	−0.0059 (4)
C1	0.0191 (6)	0.0163 (6)	0.0209 (6)	0.0011 (5)	−0.0032 (5)	−0.0048 (5)
C2	0.0219 (6)	0.0229 (6)	0.0194 (6)	0.0010 (5)	−0.0007 (5)	−0.0058 (5)
C3	0.0204 (6)	0.0189 (6)	0.0191 (6)	0.0046 (5)	−0.0051 (5)	−0.0054 (5)
C4	0.0275 (7)	0.0217 (7)	0.0246 (7)	0.0050 (5)	−0.0084 (5)	−0.0114 (5)
C5	0.0258 (7)	0.0187 (6)	0.0311 (7)	−0.0003 (5)	−0.0093 (5)	−0.0075 (5)
C6	0.0219 (6)	0.0200 (6)	0.0270 (7)	−0.0009 (5)	−0.0021 (5)	−0.0030 (5)
C7	0.0227 (6)	0.0202 (6)	0.0221 (6)	0.0022 (5)	−0.0016 (5)	−0.0064 (5)
C8	0.0202 (6)	0.0155 (6)	0.0193 (6)	0.0033 (5)	−0.0053 (5)	−0.0046 (5)
C9	0.0211 (6)	0.0180 (6)	0.0202 (6)	−0.0061 (5)	0.0031 (5)	−0.0073 (5)
C10	0.0219 (6)	0.0259 (7)	0.0234 (7)	0.0000 (5)	−0.0051 (5)	−0.0081 (5)
C11	0.0194 (6)	0.0233 (7)	0.0273 (7)	0.0020 (5)	−0.0015 (5)	−0.0099 (5)
C12	0.0266 (6)	0.0158 (6)	0.0197 (6)	−0.0059 (5)	−0.0002 (5)	−0.0037 (5)
C13	0.0314 (7)	0.0206 (7)	0.0278 (7)	0.0010 (5)	−0.0120 (6)	−0.0062 (5)
C14	0.0228 (6)	0.0174 (6)	0.0336 (7)	0.0013 (5)	−0.0060 (5)	−0.0088 (5)
C15	0.0395 (8)	0.0260 (7)	0.0221 (7)	−0.0036 (6)	−0.0014 (6)	−0.0083 (6)

Geometric parameters (Å, º)

O1—C1	1.3606 (14)	C7—C8	1.4072 (17)
O1—C9	1.4112 (14)	C7—H7	0.9500
N1—C2	1.3010 (16)	C9—C10	1.3765 (18)
N1—C3	1.3776 (16)	C9—C14	1.3774 (18)
N2—C1	1.2954 (15)	C10—C11	1.3894 (17)
N2—C8	1.3777 (15)	C10—H10	0.9500

C1—C2	1.4285 (17)	C11—C12	1.3877 (18)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.4080 (17)	C12—C13	1.3898 (18)
C3—C8	1.4159 (17)	C12—C15	1.5057 (17)
C4—C5	1.3701 (18)	C13—C14	1.3860 (18)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.4046 (18)	C14—H14	0.9500
C5—H5	0.9500	C15—H15A	0.9800
C6—C7	1.3717 (17)	C15—H15B	0.9800
C6—H6	0.9500	C15—H15C	0.9800

C1—O1—C9	117.73 (9)	C7—C8—C3	119.03 (11)
C2—N1—C3	116.77 (10)	C10—C9—C14	121.60 (12)
C1—N2—C8	115.51 (10)	C10—C9—O1	120.33 (11)
N2—C1—O1	121.46 (10)	C14—C9—O1	117.94 (11)
N2—C1—C2	123.85 (11)	C9—C10—C11	118.64 (11)
O1—C1—C2	114.69 (10)	C9—C10—H10	120.7
N1—C2—C1	121.82 (11)	C11—C10—H10	120.7
N1—C2—H2	119.1	C12—C11—C10	121.49 (11)
C1—C2—H2	119.1	C12—C11—H11	119.3
N1—C3—C4	119.73 (11)	C10—C11—H11	119.3
N1—C3—C8	120.60 (11)	C11—C12—C13	117.97 (11)
C4—C3—C8	119.67 (11)	C11—C12—C15	121.39 (11)
C5—C4—C3	120.09 (12)	C13—C12—C15	120.63 (11)
C5—C4—H4	120.0	C14—C13—C12	121.48 (12)
C3—C4—H4	120.0	C14—C13—H13	119.3
C4—C5—C6	120.34 (11)	C12—C13—H13	119.3
C4—C5—H5	119.8	C9—C14—C13	118.74 (11)
C6—C5—H5	119.8	C9—C14—H14	120.6
C7—C6—C5	120.65 (11)	C13—C14—H14	120.6
C7—C6—H6	119.7	C12—C15—H15A	109.5
C5—C6—H6	119.7	C12—C15—H15B	109.5
C6—C7—C8	120.23 (11)	H15A—C15—H15B	109.5
C6—C7—H7	119.9	C12—C15—H15C	109.5
C8—C7—H7	119.9	H15A—C15—H15C	109.5
N2—C8—C7	119.52 (11)	H15B—C15—H15C	109.5
N2—C8—C3	121.45 (11)		

C8—N2—C1—O1	−179.56 (9)	C6—C7—C8—C3	−0.28 (17)
C8—N2—C1—C2	−0.09 (17)	N1—C3—C8—N2	0.09 (17)
C9—O1—C1—N2	0.45 (16)	C4—C3—C8—N2	−179.94 (10)
C9—O1—C1—C2	−179.07 (10)	N1—C3—C8—C7	179.79 (10)
C3—N1—C2—C1	0.04 (17)	C4—C3—C8—C7	−0.23 (17)
N2—C1—C2—N1	0.07 (19)	C1—O1—C9—C10	−75.16 (14)
O1—C1—C2—N1	179.57 (10)	C1—O1—C9—C14	108.80 (12)
C2—N1—C3—C4	179.91 (10)	C14—C9—C10—C11	−2.43 (18)
C2—N1—C3—C8	−0.11 (16)	O1—C9—C10—C11	−178.32 (10)
N1—C3—C4—C5	−179.65 (10)	C9—C10—C11—C12	0.18 (18)

C8—C3—C4—C5	0.37 (18)	C10—C11—C12—C13	1.90 (18)
C3—C4—C5—C6	0.00 (18)	C10—C11—C12—C15	−178.87 (11)
C4—C5—C6—C7	−0.53 (19)	C11—C12—C13—C14	−1.86 (18)
C5—C6—C7—C8	0.67 (18)	C15—C12—C13—C14	178.91 (11)
C1—N2—C8—C7	−179.68 (10)	C10—C9—C14—C13	2.47 (18)
C1—N2—C8—C3	0.02 (16)	O1—C9—C14—C13	178.45 (10)
C6—C7—C8—N2	179.42 (10)	C12—C13—C14—C9	−0.27 (18)