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2,5-Dimethylphenyl quinoline-2-carboxylate

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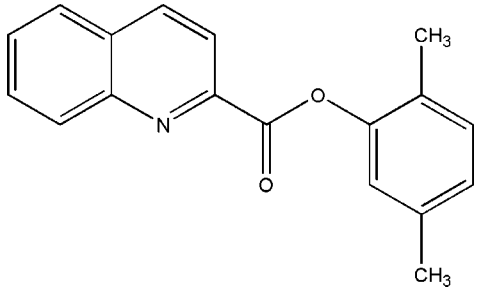
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.101; data-to-parameter ratio = 14.1.

In the title compound, $C_{18}H_{15}NO_2$, the dihedral angle between the mean planes of the quinoline ring system and the phenyl ring is 78.8 (1)°. The mean plane of the carboxylate group is twisted from the mean planes of the quinoline ring system and phenyl ring by 1.5 (9) and 77.6 (4)°, respectively. In the crystal, molecules are linked by weak C—H···O interactions, generating $C(8)$ chains along [001]. Weak π–π stacking interactions are also observed [centroid–centroid separation = 3.6238 (12) Å].

Related literature

For related structures and background to quinoline derivatives, see: Fazal *et al.* (2014); Jasinski *et al.* (2010).



Experimental

Crystal data

$C_{18}H_{15}NO_2$ M_r = 277.31
Orthorhombic, $P2_12_12_1$
a = 8.2261 (3) Å
b = 11.6007 (5) Å
c = 14.5738 (5) Å
V = 1390.76 (9) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 173 K
0.46 × 0.34 × 0.18 mm

Data collection

Agilent Gemini EOS diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.711, T_{max} = 1.000
8332 measured reflections
2721 independent reflections
2585 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.05
2721 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack parameter determined using 1049 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.04 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17B···O1^{i}	0.98	2.49	3.389 (3)	152

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

EF thanks the CFTRI, Mysore and Yuvaraja's College, UOM, for providing research facilities. EF is grateful to Mr J. R. Manjunatha, PPSFT, CFTRI for the NMR spectra. JPJ acknowledges the NSF–MRI program (grant No. CHE-1039027) for funds to purchase the X-ray diffractometer.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7183).

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supporting information

Acta Cryst. (2014). E**70**, o147 [doi:10.1107/S160053681400052X]

2,5-Dimethylphenyl quinoline-2-carboxylate

E. Fazal, Manpreet Kaur, Jerry P. Jasinski, S. Nagarajan and B. S. Sudha

S1. Comment

Following our recent report on 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate (Fazal *et al.*, 2014), we now describe the crystal structure of the title compound, (I), The synthesis, crystal structures and theoretical studies of four Schiff bases derived from 4-hydrazinyl-8-(trifluoromethyl) quinoline (Jasinski *et al.*, 2010) have also been reported.

The dihedral angle between the mean planes of the quinoline ring and the phenyl ring is 78.8 (1)° (Fig. 1). The mean plane of the carboxylate group is twisted from the mean planes of the quinoline ring and phenyl ring by 1.5 (9)° and 77.6 (4)°, respectively. The crystal packing is influenced by weak C17—H17B···O1 interactions making chains along [0 0 1](Fig. 2). In addition, weak Cg2–Cg3 π–π interactions are observed (Cg2–Cg3 = 3.6238 (12)Å; Cg2 = C5–C10; Cg3 = C11–C16; 1/2 + x, 1/2 - y, 1 - z).

S2. Experimental

To a mixture of 1.73 g (10 mmole) of quinaldic acid and 1.56 g (10 mmole) of 2,5-dimethylphenol in a round-bottomed flask fitted with a reflux condenser with a drying tube was added 0.15 g (10 mmole) of phosphorous oxychloride. The mixture was heated with occasional swirling, and temperature maintained at 348-353 K. At the end of eight hours the reaction mixture was poured in to a solution of 2 g of sodium bicarbonate in 25 ml of water. The precipitated ester was collected on a filter and washed with water. The yield of crude, air dried 2,5-dimethylphenyl quinoline-2-carboxylate was 1.71 to 1.85 g (65-70 %). Irregular colourless chunks were obtained by recrystallization from absolute ethanol solution by slow evaporation.

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.95Å (CH) or 0.98Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.2 (CH) or 1.5 (CH_3) times U_{eq} of the parent atom. Idealised Me refined as rotating group.

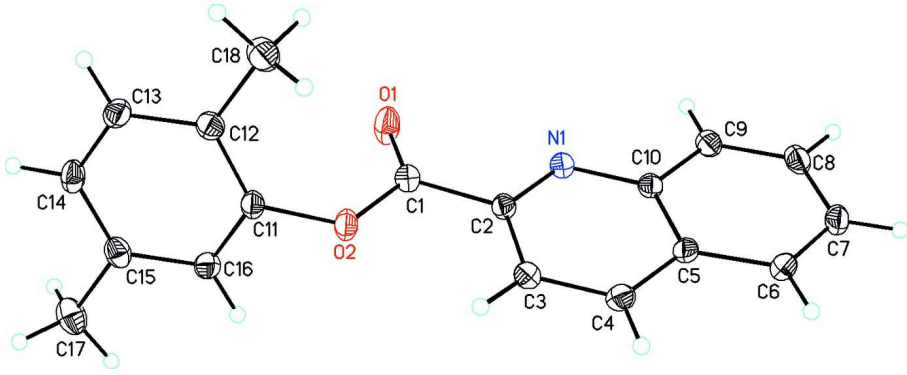

Figure 1

ORTEP drawing of (I) ($C_{18}H_{15}NO_2$) showing 30% probability displacement ellipsoids.

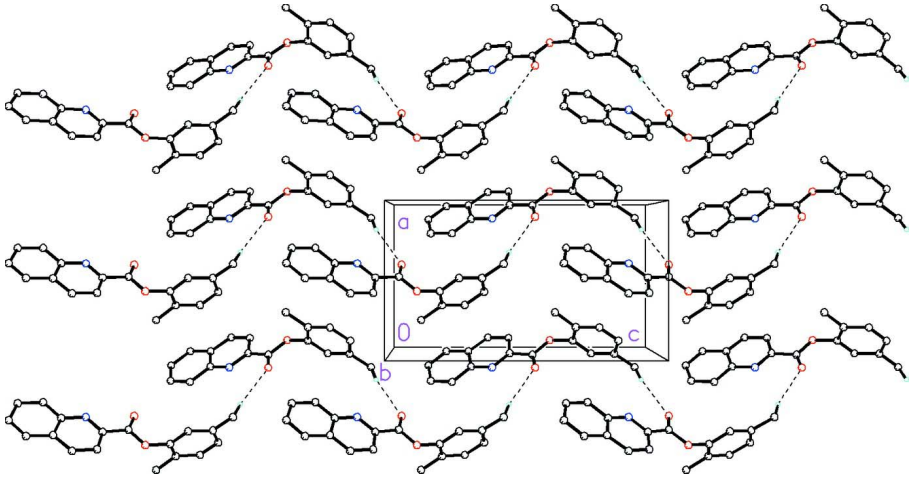

Figure 2

Molecular packing for (I) viewed along the *b* axis. Dashed lines indicate weak C17—H17B···O1 intermolecular interactions making chains along [0 0 1] and influence the crystal packing. The remaining H atoms have been removed for clarity.

2,5-Dimethylphenyl quinoline-2-carboxylate

Crystal data

$C_{18}H_{15}NO_2$
M_r = 277.31
Orthorhombic, $P2_12_12_1$
a = 8.2261 (3) Å
b = 11.6007 (5) Å
c = 14.5738 (5) Å
V = 1390.76 (9) Å^3
Z = 4
$F(000)$ = 584

D_x = 1.324 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3982 reflections
θ = 3.0–72.4°
μ = 0.69 mm^{-1}
T = 173 K
Irregular, colourless
0.46 × 0.34 × 0.18 mm

Data collection

Agilent Gemini EOS diffractometer
Radiation source: Enhance (Cu) X-ray Source

Detector resolution: 16.0416 pixels mm^{-1}
ω scans

Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.711, T_{max} = 1.000
8332 measured reflections
2721 independent reflections
2585 reflections with $I > 2\sigma(I)$

R_{int} = 0.031
θ_{max} = 72.6°, θ_{min} = 4.9°
h = −6→10
k = −14→13
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.05
2721 reflections
193 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.1748P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL2012* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0027 (7)
Absolute structure: Flack parameter determined using 1049 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.04 (16)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.4090 (2)	0.00776 (14)	0.45505 (11)	0.0439 (4)
O2	0.5803 (2)	0.13777 (12)	0.39481 (9)	0.0330 (4)
N1	0.3984 (2)	0.13265 (14)	0.61466 (11)	0.0259 (4)
C1	0.4863 (2)	0.09441 (16)	0.46254 (13)	0.0274 (4)
C2	0.4902 (2)	0.16990 (15)	0.54669 (12)	0.0248 (4)
C3	0.5847 (2)	0.27162 (16)	0.54988 (13)	0.0276 (4)
H3	0.6468	0.2956	0.4984	0.033*
C4	0.5840 (3)	0.33438 (17)	0.62920 (14)	0.0292 (4)
H4	0.6464	0.4031	0.6334	0.035*
C5	0.4907 (3)	0.29728 (16)	0.70485 (13)	0.0265 (4)
C6	0.4872 (3)	0.35546 (17)	0.79056 (14)	0.0321 (4)
H6	0.5502	0.4232	0.7992	0.038*
C7	0.3934 (3)	0.31404 (19)	0.86066 (14)	0.0349 (5)
H7	0.3927	0.3529	0.9180	0.042*
C8	0.2979 (3)	0.21456 (19)	0.84884 (14)	0.0334 (5)
H8	0.2323	0.1877	0.8981	0.040*
C9	0.2982 (3)	0.15600 (17)	0.76741 (14)	0.0296 (4)
H9	0.2325	0.0893	0.7601	0.035*
C10	0.3968 (2)	0.19518 (16)	0.69387 (13)	0.0252 (4)
C11	0.5828 (2)	0.07494 (17)	0.31151 (12)	0.0271 (4)

C12	0.6794 (2)	−0.02221 (17)	0.30398 (14)	0.0286 (4)
C13	0.6803 (3)	−0.07618 (18)	0.21885 (14)	0.0318 (4)
H13	0.7445	−0.1435	0.2107	0.038*
C14	0.5903 (3)	−0.03456 (18)	0.14550 (14)	0.0326 (5)
H14	0.5932	−0.0740	0.0884	0.039*
C15	0.4960 (2)	0.06388 (18)	0.15446 (13)	0.0313 (4)
C16	0.4932 (3)	0.11850 (17)	0.23933 (14)	0.0294 (4)
H16	0.4294	0.1860	0.2477	0.035*
C17	0.4019 (3)	0.1117 (2)	0.07440 (16)	0.0452 (6)
H17A	0.3427	0.1809	0.0938	0.068*
H17B	0.3245	0.0537	0.0525	0.068*
H17C	0.4772	0.1318	0.0248	0.068*
C18	0.7792 (3)	−0.0662 (2)	0.38316 (16)	0.0400 (5)
H18A	0.8297	−0.0011	0.4151	0.060*
H18B	0.8640	−0.1180	0.3601	0.060*
H18C	0.7088	−0.1083	0.4258	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0543 (10)	0.0445 (9)	0.0330 (8)	−0.0212 (8)	0.0128 (8)	−0.0122 (7)
O2	0.0444 (8)	0.0311 (7)	0.0235 (7)	−0.0073 (6)	0.0076 (6)	−0.0061 (5)
N1	0.0281 (8)	0.0265 (8)	0.0232 (8)	0.0012 (7)	0.0003 (7)	−0.0005 (6)
C1	0.0283 (9)	0.0294 (9)	0.0246 (9)	−0.0001 (8)	0.0006 (8)	−0.0011 (7)
C2	0.0270 (8)	0.0262 (9)	0.0211 (8)	0.0032 (8)	−0.0015 (8)	−0.0008 (7)
C3	0.0305 (9)	0.0273 (9)	0.0251 (9)	0.0009 (8)	0.0008 (8)	0.0019 (7)
C4	0.0327 (9)	0.0237 (9)	0.0311 (10)	−0.0010 (8)	−0.0015 (8)	−0.0002 (8)
C5	0.0308 (9)	0.0238 (9)	0.0248 (9)	0.0061 (8)	−0.0032 (8)	−0.0015 (7)
C6	0.0415 (11)	0.0251 (9)	0.0296 (10)	0.0033 (9)	−0.0039 (9)	−0.0041 (7)
C7	0.0453 (11)	0.0359 (11)	0.0234 (9)	0.0113 (10)	−0.0012 (9)	−0.0056 (8)
C8	0.0372 (10)	0.0397 (11)	0.0232 (9)	0.0093 (9)	0.0029 (9)	0.0028 (8)
C9	0.0302 (9)	0.0321 (10)	0.0264 (10)	0.0025 (8)	−0.0001 (8)	0.0021 (8)
C10	0.0269 (9)	0.0255 (9)	0.0234 (8)	0.0052 (8)	−0.0015 (7)	0.0004 (7)
C11	0.0336 (10)	0.0254 (9)	0.0222 (8)	−0.0067 (8)	0.0048 (8)	−0.0033 (7)
C12	0.0289 (9)	0.0281 (9)	0.0288 (10)	−0.0035 (8)	0.0038 (8)	0.0017 (8)
C13	0.0338 (10)	0.0272 (9)	0.0344 (10)	−0.0004 (9)	0.0087 (9)	−0.0026 (8)
C14	0.0377 (10)	0.0345 (11)	0.0256 (9)	−0.0093 (9)	0.0046 (9)	−0.0091 (8)
C15	0.0300 (9)	0.0375 (10)	0.0263 (9)	−0.0080 (9)	0.0015 (9)	0.0012 (8)
C16	0.0316 (9)	0.0271 (9)	0.0296 (10)	0.0012 (9)	0.0056 (8)	0.0005 (7)
C17	0.0443 (12)	0.0608 (15)	0.0306 (11)	−0.0007 (12)	−0.0047 (10)	0.0035 (10)
C18	0.0411 (12)	0.0450 (12)	0.0338 (11)	0.0028 (10)	0.0004 (10)	0.0049 (10)

Geometric parameters (Å, º)

O1—C1	1.194 (2)	C9—H9	0.9500
O2—C1	1.351 (2)	C9—C10	1.419 (3)
O2—C11	1.416 (2)	C11—C12	1.383 (3)
N1—C2	1.319 (2)	C11—C16	1.380 (3)

N1—C10	1.363 (2)	C12—C13	1.390 (3)
C1—C2	1.507 (2)	C12—C18	1.505 (3)
C2—C3	1.414 (3)	C13—H13	0.9500
C3—H3	0.9500	C13—C14	1.387 (3)
C3—C4	1.366 (3)	C14—H14	0.9500
C4—H4	0.9500	C14—C15	1.387 (3)
C4—C5	1.411 (3)	C15—C16	1.390 (3)
C5—C6	1.420 (2)	C15—C17	1.507 (3)
C5—C10	1.423 (3)	C16—H16	0.9500
C6—H6	0.9500	C17—H17A	0.9800
C6—C7	1.368 (3)	C17—H17B	0.9800
C7—H7	0.9500	C17—H17C	0.9800
C7—C8	1.407 (3)	C18—H18A	0.9800
C8—H8	0.9500	C18—H18B	0.9800
C8—C9	1.367 (3)	C18—H18C	0.9800

C1—O2—C11	116.31 (15)	C9—C10—C5	119.47 (17)
C2—N1—C10	117.84 (16)	C12—C11—O2	119.72 (17)
O1—C1—O2	123.44 (18)	C16—C11—O2	117.19 (17)
O1—C1—C2	125.08 (18)	C16—C11—C12	123.00 (17)
O2—C1—C2	111.47 (16)	C11—C12—C13	116.18 (18)
N1—C2—C1	114.13 (16)	C11—C12—C18	121.93 (18)
N1—C2—C3	124.32 (17)	C13—C12—C18	121.89 (19)
C3—C2—C1	121.55 (17)	C12—C13—H13	119.1
C2—C3—H3	121.0	C14—C13—C12	121.88 (19)
C4—C3—C2	118.05 (18)	C14—C13—H13	119.1
C4—C3—H3	121.0	C13—C14—H14	119.6
C3—C4—H4	120.0	C15—C14—C13	120.84 (18)
C3—C4—C5	120.07 (18)	C15—C14—H14	119.6
C5—C4—H4	120.0	C14—C15—C16	117.95 (19)
C4—C5—C6	123.59 (18)	C14—C15—C17	121.20 (19)
C4—C5—C10	117.47 (16)	C16—C15—C17	120.8 (2)
C6—C5—C10	118.93 (17)	C11—C16—C15	120.15 (19)
C5—C6—H6	120.0	C11—C16—H16	119.9
C7—C6—C5	120.08 (19)	C15—C16—H16	119.9
C7—C6—H6	120.0	C15—C17—H17A	109.5
C6—C7—H7	119.6	C15—C17—H17B	109.5
C6—C7—C8	120.80 (18)	C15—C17—H17C	109.5
C8—C7—H7	119.6	H17A—C17—H17B	109.5
C7—C8—H8	119.6	H17A—C17—H17C	109.5
C9—C8—C7	120.9 (2)	H17B—C17—H17C	109.5
C9—C8—H8	119.6	C12—C18—H18A	109.5
C8—C9—H9	120.1	C12—C18—H18B	109.5
C8—C9—C10	119.82 (19)	C12—C18—H18C	109.5
C10—C9—H9	120.1	H18A—C18—H18B	109.5
N1—C10—C5	122.21 (17)	H18A—C18—H18C	109.5
N1—C10—C9	118.32 (17)	H18B—C18—H18C	109.5

O1—C1—C2—N1	−0.1 (3)	C6—C5—C10—C9	2.1 (3)
O1—C1—C2—C3	−179.8 (2)	C6—C7—C8—C9	0.9 (3)
O2—C1—C2—N1	178.98 (16)	C7—C8—C9—C10	0.5 (3)
O2—C1—C2—C3	−0.7 (3)	C8—C9—C10—N1	177.87 (18)
O2—C11—C12—C13	−177.39 (17)	C8—C9—C10—C5	−1.9 (3)
O2—C11—C12—C18	2.0 (3)	C10—N1—C2—C1	179.07 (16)
O2—C11—C16—C15	177.19 (17)	C10—N1—C2—C3	−1.3 (3)
N1—C2—C3—C4	1.5 (3)	C10—C5—C6—C7	−0.8 (3)
C1—O2—C11—C12	−79.9 (2)	C11—O2—C1—O1	0.5 (3)
C1—O2—C11—C16	103.4 (2)	C11—O2—C1—C2	−178.63 (15)
C1—C2—C3—C4	−178.88 (17)	C11—C12—C13—C14	0.3 (3)
C2—N1—C10—C5	−0.3 (3)	C12—C11—C16—C15	0.6 (3)
C2—N1—C10—C9	179.87 (17)	C12—C13—C14—C15	0.5 (3)
C2—C3—C4—C5	−0.1 (3)	C13—C14—C15—C16	−0.8 (3)
C3—C4—C5—C6	177.96 (18)	C13—C14—C15—C17	178.1 (2)
C3—C4—C5—C10	−1.4 (3)	C14—C15—C16—C11	0.2 (3)
C4—C5—C6—C7	179.9 (2)	C16—C11—C12—C13	−0.9 (3)
C4—C5—C10—N1	1.6 (3)	C16—C11—C12—C18	178.5 (2)
C4—C5—C10—C9	−178.58 (18)	C17—C15—C16—C11	−178.65 (19)
C5—C6—C7—C8	−0.7 (3)	C18—C12—C13—C14	−179.00 (19)
C6—C5—C10—N1	−177.74 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*B*···O1^{i}	0.98	2.49	3.389 (3)	152

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