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2-Methyl-3-(2-methylphenyl)-4-oxo-3,4-dihydroquinazolin-8-yl benzoate

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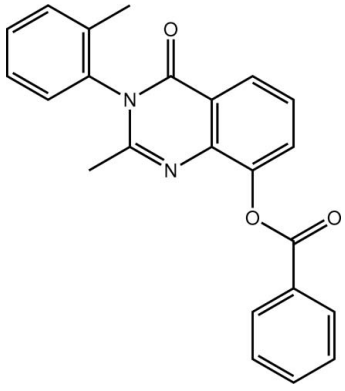
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.132; data-to-parameter ratio = 14.8.

In the title quinazolin-4-one derivative, $C_{23}H_{18}N_2O_3$, both the benzoate [dihedral angle = 79.99 (6)°] and the 2-tolyl [89.02 (7)°] groups are close to orthogonal to the central fused ring system. Both aryl groups are orientated towards the quinazolin-4-one-bound methyl group. In the crystal, molecules are connected into a three-dimensional architecture by C—H···O, C—H···N and C—H···π interactions.

Related literature

For the pharmacological activity of substituted quinazoline-4(3*H*)-ones, see: El-Azab & El-Tahir (2012); El-Azab *et al.* (2011); Al-Omary *et al.* (2010); Al-Obaid *et al.* (2009); Aziza *et al.* (1996). For the synthesis and evaluation of the anti-convulsant activity of the title compound, see: El-Azab *et al.* (2010). For the structure of the benzoate derivative, see: El-Azab *et al.* (2012).



Experimental

Crystal data

$C_{23}H_{18}N_2O_3$
M_r = 370.39
Monoclinic, $P2_1/c$
a = 20.3847 (4) Å
b = 7.4352 (1) Å
c = 12.7829 (3) Å
β = 107.489 (2)°
V = 1847.87 (6) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 100 K
0.30 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.470, T_{max} = 1.000
7377 measured reflections
3780 independent reflections
3432 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.132
S = 1.05
3780 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

*Cg*1 is the centroid of the C17–C22 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	0.95	2.58	3.521 (2)	172
C16—H16c···O2^{ii}	0.98	2.44	3.298 (2)	146
C20—H20···O3^{iii}	0.95	2.59	3.225 (2)	124
C11—H11···*Cg*1^{iv}	0.95	2.72	3.5519 (18)	147

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, y+1, z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6635).

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