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

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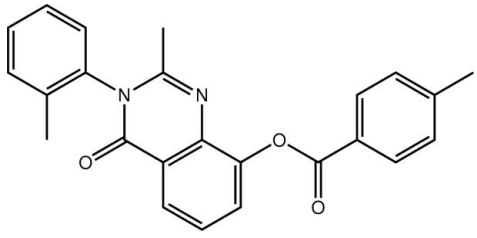
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.067; wR factor = 0.186; data-to-parameter ratio = 14.7.

In the title quinazolin-4-one derivative, $C_{24}H_{20}N_2O_3$, both the 4-methylbenzoate [dihedral angle = 83.90 (9)°] and 2-tolyl [87.88 (9)°] groups are almost orthogonal to the central fused ring system. These aryl groups are oriented 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···π and π–π [ring centroid-to-centroid separation = 3.6458 (13) Å] interactions.

Related literature

For the pharmacological activity of substituted quinazoline-4(3*H*)-ones, see: El-Azab & ElTahir (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

$C_{24}H_{20}N_2O_3$
M_r = 384.42
Monoclinic, $P2_1/c$
a = 18.8216 (5) Å
b = 7.6332 (2) Å
c = 13.3092 (3) Å
β = 97.286 (2)°
V = 1896.68 (8) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.755, T_{max} = 1.000
7966 measured reflections
3883 independent reflections
3478 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.186
S = 1.06
3883 reflections
265 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

*Cg*1 is the centroid of the C18–C23 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17*C*···O2^{i}	0.98	2.55	3.434 (3)	150
C21—H21···O3^{ii}	0.95	2.47	3.299 (3)	146
C12—H12···*Cg*1^{iii}	0.95	2.79	3.658 (2)	153

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

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: HB6636).

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