

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2,2'-Bis(4-fluoroanilino)-3,3'-(3,6-dioxaoctane-1,8-diyl)diquinazolin-4(3H)-one

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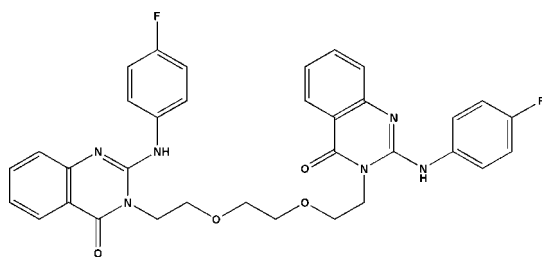
Received 10 November 2008; accepted 3 December 2008

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.048; wR factor = 0.146; data-to-parameter ratio = 13.6.

In the centrosymmetric title compound, $\text{C}_{34}\text{H}_{30}\text{F}_2\text{N}_6\text{O}_4$, the dihedral angle between the quinazolinone and fluorobenzene ring planes are 71.00 (2) and 74.94 (2)° and an intramolecular $\text{N}-\text{H}\cdots\text{O}$ interaction stabilizes the conformation. In the crystal, $\text{C}-\text{H}\cdots\text{F}$ and $\text{C}-\text{H}\cdots\text{O}$ links help to establish the packing.

Related literature

For the biological activity of quinazolinones, see: Shiba *et al.* (1997); Ding *et al.*, 2004. For the crystal structures of other fused heterocyclic derivatives, see: Wang *et al.* (2006); Xu *et al.* (2006).



Experimental

Crystal data

$\text{C}_{34}\text{H}_{30}\text{F}_2\text{N}_6\text{O}_4$
 $M_r = 624.64$

Monoclinic, $C2/c$
 $a = 13.923$ (3) Å

$b = 12.509$ (3) Å
 $c = 18.726$ (4) Å
 $\beta = 97.08$ (3)°
 $V = 3236.6$ (11) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 295$ (2) K
 $0.20 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.982$, $T_{\max} = 0.991$

2834 measured reflections
2834 independent reflections
2263 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.0123$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.146$
 $S = 1.06$
2834 reflections

208 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.30$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O2}$	0.86	2.18	2.7954 (19)	128
$\text{C16}-\text{H16A}\cdots\text{F1}^{\text{i}}$	0.97	2.54	3.388 (2)	146
$\text{C16}-\text{H16B}\cdots\text{O1}^{\text{ii}}$	0.97	2.43	3.377 (2)	164

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

We thank Dr Xiang-Gao Meng for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2676).

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