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3,3,6,6-Tetramethyl-9-[6-(3,3,6,6-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1*H*-xanthen-9-yl)pyridin-2-yl]-2,3,4,5,6,7,8,9-octahydro-1*H*-xanthene-1,8-dione

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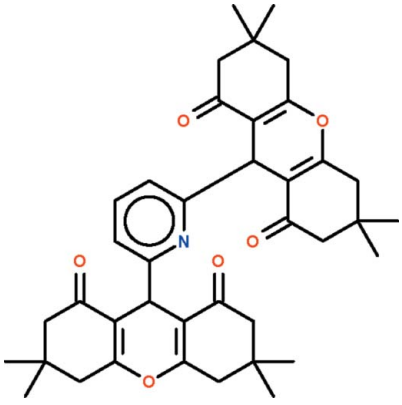
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.111; data-to-parameter ratio = 18.6.

In the title molecule, $C_{39}H_{45}NO_6$, the two tetramethyloctahydroxanthen-1,8-dione substituents are arranged approximately parallel to each other and approximately perpendicular to the plane of the pyridine ring. The six-membered xanthene rings adopt flattened boat conformations with the O and methine C atoms deviating from the plane of the other four atoms.

Related literature

For a related structure, see: Mohamed *et al.* (2011).



Experimental

Crystal data

$C_{39}H_{45}NO_6$
M_r = 623.76
Monoclinic, $P2_1/c$
a = 24.1384 (8) Å
b = 10.0371 (4) Å
c = 14.4408 (5) Å
β = 105.8460 (7)°
V = 3365.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.30 × 0.30 × 0.30 mm

Data collection

Bruker APEXII diffractometer
35921 measured reflections
7717 independent reflections
6410 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
S = 1.03
7717 reflections
415 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5213).

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