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Dimethyl 2,2′-[(4-oxo-2-phenyl-4*H*-chromene-5,7-diyl)dioxy]diacetate: a less densely packed polymorph

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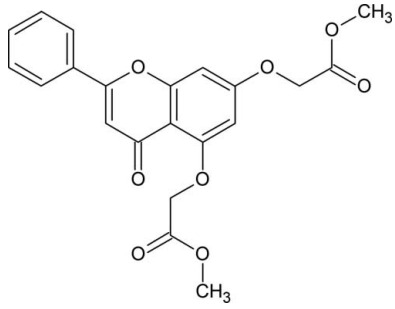
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.140; data-to-parameter ratio = 16.3.

The title molecule, $C_{21}H_{18}O_8$, crystallizes in two crystal polymorphs, see also Nallasivam, Nethaji, Vembu & Jaswant [*Acta Cryst.* (2009), E**65**, o312–o313]. The main difference between the two polymorphs is in the conformation of the oxomethylacetate groups with regard to the almost planar [total puckering amplitude 0.047 (2) Å] chromene ring. In the title compound, the best planes of the oxomethylacetate groups through the non-H atoms are almost perpendicular to the chromene ring [making dihedral angles of 89.61 (6) and 80.59 (5)°], while in the second polymorph the molecules are close to planar. Both crystal structures are stabilized by C—H···O.

Related literature

For the second polymorph, see: Nallasivam *et al.* (2009). For the biological and pharmacological properties of benzopyrans and their derivatives, see: Brooks (1998); Hatakeyama *et al.* (1988); Hyana & Saimoto (1987); Tang *et al.* (2007). For the importance of 4*H*-chromenes, see Liu *et al.* (2007); Wang, Fang *et al.* (2003); Wand, Zheng *et al.* (2003).For hydrogen-bond motifs, see: Bernstein *et al.* (1995); Desiraju & Steiner (1999); Etter (1990).



Experimental

Crystal data

$C_{21}H_{18}O_8$
M_r = 398.35
Triclinic, $P\overline{1}$
a = 9.4024 (16) Å
b = 9.8506 (17) Å
c = 11.1570 (18) Å
α = 67.817 (3)°
β = 80.300 (3)°
γ = 89.683 (3)°
V = 941.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
0.42 × 0.35 × 0.29 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.955, T_{max} = 0.969
8351 measured reflections
4316 independent reflections
2424 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.140
S = 0.98
4316 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19A···O17^{i}	0.97	2.54	3.214 (3)	127
C19—H19A···O18^{i}	0.97	2.58	3.366 (2)	138

Symmetry codes: (i) $-x+1, -y+1, -z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2124).

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