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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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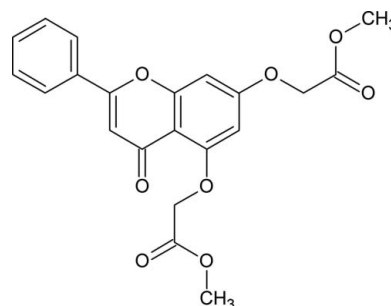
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.055; wR factor = 0.140; data-to-parameter ratio = 16.3.

The title molecule, $\text{C}_{21}\text{H}_{18}\text{O}_8$, crystallizes in two crystal polymorphs, see also Nallasivam, Nethaji, Vembu & Jaswant [*Acta Cryst.* (2009), **E65**, 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 $\text{C}-\text{H}\cdots\text{O}$.

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

$\text{C}_{21}\text{H}_{18}\text{O}_8$
 $M_r = 398.35$
Triclinic, $P\bar{1}$
 $a = 9.4024$ (16) Å
 $b = 9.8506$ (17) Å
 $c = 11.1570$ (18) Å
 $\alpha = 67.817$ (3)°
 $\beta = 80.300$ (3)°
 $\gamma = 89.683$ (3)°
 $V = 941.3$ (3) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.11$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

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
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C19}-\text{H19A}\cdots\text{O17}^i$	0.97	2.54	3.214 (3)	127
$\text{C19}-\text{H19A}\cdots\text{O18}^i$	0.97	2.58	3.366 (2)	138

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; 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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