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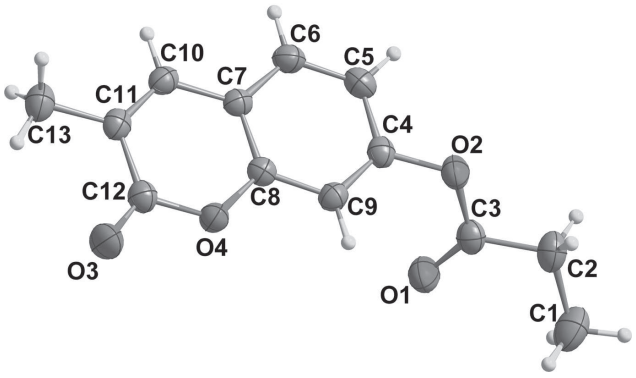
Crystal structure of 3-methyl-2-oxo-2*H*-chromen-7-yl propionate, $C_{13}H_{12}O_4$



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Abstract

$C_{13}H_{12}O_4$, triclinic, $P\bar{1}$ (no. 2), $a = 6.141(5)$ Å, $b = 8.108(6)$ Å, $c = 12.234(9)$ Å, $\alpha = 79.257(12)°$, $\beta = 76.820(12)°$, $\gamma = 74.687(11)°$, $V = 566.8(7)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0515$, $wR_{ref}(F^2) = 0.1575$, $T = 296(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was synthesized according to the literature method [3]. Crystals suitable for X-ray diffraction analysis were obtained via recrystallization from an ethanol solution.

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [1]. The hydro-

Table 1: Data collection and handling.

Crystal:	Colourless rod
Size:	0.20 × 0.12 × 0.08 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.10 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2893, 1990, 0.011
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1556
$N(param)_{refined}$:	154
Programs:	SHELX [1], Bruker [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
O1	0.2510(3)	0.0298(2)	0.85649(15)	0.0751(6)
O2	0.0494(3)	−0.12022(19)	0.79958(13)	0.0610(5)
O3	0.4041(3)	0.3615(3)	0.29128(15)	0.0809(6)
O4	0.2805(2)	0.22045(19)	0.45430(12)	0.0540(4)
C1	0.4215(6)	−0.2544(4)	1.0112(3)	0.0959(10)
H1A	0.444679	−0.357035	1.065020	0.144*
H1B	0.561221	−0.251871	0.956954	0.144*
H1C	0.379030	−0.154790	1.050098	0.144*
C2	0.2340(5)	−0.2536(3)	0.9515(2)	0.0722(7)
H2A	0.276733	−0.356084	0.913999	0.087*
H2B	0.094638	−0.259054	1.007094	0.087*
C3	0.1860(4)	−0.0993(3)	0.86638(18)	0.0553(6)
C4	−0.0021(4)	0.0090(3)	0.71067(17)	0.0496(5)
C5	−0.2322(4)	0.0800(3)	0.70763(19)	0.0565(6)
H5A	−0.345748	0.047562	0.766009	0.068*
C6	−0.2902(4)	0.1988(3)	0.6171(2)	0.0567(6)
H6A	−0.444486	0.246220	0.614149	0.068*
C7	−0.1222(3)	0.2496(2)	0.52984(17)	0.0459(5)
C8	0.1062(3)	0.1751(2)	0.53752(16)	0.0442(5)
C9	0.1691(4)	0.0535(3)	0.62614(17)	0.0490(5)
H9A	0.322999	0.003177	0.628561	0.059*
C10	−0.1680(4)	0.3680(3)	0.43092(19)	0.0523(5)
H10A	−0.319884	0.416951	0.423622	0.063*
C11	0.0003(4)	0.4105(3)	0.34860(18)	0.0510(5)
C12	0.2373(4)	0.3343(3)	0.35891(18)	0.0543(5)
C13	−0.0395(5)	0.5291(3)	0.2426(2)	0.0692(7)
H13A	0.105616	0.540856	0.195891	0.104*
H13B	−0.121520	0.482765	0.202191	0.104*
H13C	−0.128268	0.640215	0.261331	0.104*

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gen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Comment

Coumarin is a simple flavonoid molecule and is a natural constituent of many plants and essential oils. The synthesis of methylcoumarin derivatives dates back to the beginning of the last century [4]. Coumarin derivatives have been proven to function as an anti-coagulants, antibacterial agents, antifungal agents, biological inhibitors, chemotherapeutics and as bio-analytical reagents [5, 6].

In the title structure, all bond lengths lie in the normal range and excellently fit with those derived from the crystal structure of the parent compound 3-methyl-2*H*-chromen-2-one [7]. In the crystal, pairs of weak intermolecular C—H···O hydrogen bonds link two molecules into a centrosymmetric dimers. The dimers are weakly connected with others via further C—H···O hydrogen bonds, forming a chain structure along *a*.

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