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3-Benzylidene-6-methoxychroman-4-one

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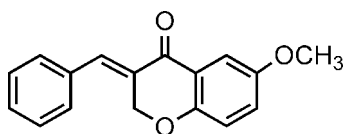
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.039; wR factor = 0.116; data-to-parameter ratio = 16.3.

In the title compound, $\text{C}_{17}\text{H}_{14}\text{O}_3$, the dihedral angle between the phenyl ring and the benzene ring of the chromanone moiety is $67.78(3)^\circ$. The six-membered heterocyclic ring of the chromanone moiety adopts a half-chair conformation. The structure is stabilized by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions that link the molecules into inversion dimers.

Related literature

For background literature, see: Finch & Tamm (1970); Geen *et al.* (1996); Tietze & Gerlitzer (1997); Cremer & Pople (1975). For a related structure, see: Suresh *et al.* (2007).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{14}\text{O}_3$
 $M_r = 266.28$
 Triclinic, $P\bar{1}$

$a = 7.2678(2)$ Å
 $b = 8.3151(2)$ Å
 $c = 11.7999(4)$ Å

$\alpha = 95.964(1)^\circ$
 $\beta = 103.828(1)^\circ$
 $\gamma = 104.042(1)^\circ$
 $V = 661.74(3)$ Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 298(2)$ K
 $0.45 \times 0.42 \times 0.38$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1999)
 $T_{\min} = 0.960$, $T_{\max} = 0.966$

8868 measured reflections
 3041 independent reflections
 2404 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.116$
 $S = 1.04$
 3041 reflections
 186 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.24$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{C6}-\text{H6}\cdots\text{O1}^i$ | 0.93 | 2.53 | 3.4293 (18) | 163 |

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

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2 (Bruker, 2004); data reduction: SAINT-Plus (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2222).

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supplementary materials

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3-Benzylidene-6-methoxychroman-4-one

T. Augustine, S. M. Vithiya, V. Ramkumar and C. C. Kanakam

Comment

The chroman-4-one (2,3-dihydro-4-oxo-4*H*-1-benzopyran) ring system occupies an important position among oxygen heterocyclics and features in a wide variety of compounds of biological and medicinal interest (Finch & Tamm, 1970). Many biologically active natural products containing a chroman ring system have been synthesized *via* 2-substituted chroman-4-one intermediates including alpha-tocopherol (vitamin E) (Geen *et al.*, 1996). 3-arylidene-4-chromanones have also been isolated as natural products belonging to the class of compounds called homoisoflavonoids (Tietze & Gerlitzer, 1997).

The geometric parameters in the title compound agree with values reported for a similar structure (Suresh *et al.*, 2007). The dihedral angle between the benzene ring of the chromanone moiety and the phenyl ring is 67.78 (3)°. The Chromanone moiety is fused with a six membered heterocyclic ring and the study of torsion angles, asymmetry parameters and least-square plane calculations shows that the chromanone adopts a half chair conformation with a deviation of C14 from the C8/C9/C15/C16/O2 plane by 0.616 (4) Å, Q₂= 0.4053 (14) Å, Q₃= -0.2052 (13) Å, and Q_T=0.4543 (14) Å (Cremer & Pople, (1975). The structure is stabilized by weak intermolecular C—H···O interaction that link the molecules into pairs around a center (Table 1). No other short intermolecular interactions were found.

Experimental

Methyl-(2*Z*)-2-bromo methyl-3-aryl prop-2-enoate (0.006 mole, 1.53 g) was treated with 4-methoxy phenol (0.006 mole, 0.9 ml) in the presence of potassium carbonate in acetone at reflux temperature for 3 hrs. The pure ester, 3-aryl-2-(4-methoxy)-phenoxyprop-2-enoate was obtained after purifying it using silica gel and column chromatography (3% ethyl acetate - hexane). Hydrolysis of this ester was carried out with KOH in aqueous 1,4-dioxane at room temperature. The reaction mixture was acidified and the precipitated acid was purified by recrystallization. Finally the acid was treated with trifluoroacetic anhydride and the reaction mixture was refluxed in dichloro- methane for 1 hr. It was further purified by column chromatography (silica gel-3% ethyl acetate - hexane) and the crystals used for data collection were obtained by slow evaporation from methanol.

Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic C—H, C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH₂, C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{iso}}(\text{C})$ for CH₃.

Figures

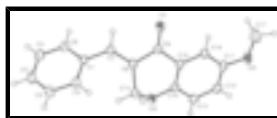


Fig. 1. ORTEP of the molecule with atoms represented as 30% probability ellipsoids.

3-Benzylidene-6-methoxychroman-4-one

Crystal data

| | |
|--------------------------------|---|
| $C_{17}H_{14}O_3$ | $Z = 2$ |
| $M_r = 266.28$ | $F_{000} = 280$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.336 \text{ Mg m}^{-3}$ |
| Hall symbol: -p 1 | Mo $K\alpha$ radiation |
| $a = 7.2678 (2) \text{ \AA}$ | $\lambda = 0.71073 \text{ \AA}$ |
| $b = 8.3151 (2) \text{ \AA}$ | Cell parameters from 4851 reflections |
| $c = 11.7999 (4) \text{ \AA}$ | $\theta = 2.6\text{--}28.3^\circ$ |
| $\alpha = 95.9640 (10)^\circ$ | $\mu = 0.09 \text{ mm}^{-1}$ |
| $\beta = 103.8280 (10)^\circ$ | $T = 298 (2) \text{ K}$ |
| $\gamma = 104.0420 (10)^\circ$ | Block, colourless |
| $V = 661.74 (3) \text{ \AA}^3$ | $0.45 \times 0.42 \times 0.38 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker APEXII CCD area-detector diffractometer | 3041 independent reflections |
| Radiation source: fine-focus sealed tube | 2404 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.018$ |
| $T = 298(2) \text{ K}$ | $\theta_{\text{max}} = 28.3^\circ$ |
| φ and ω scans | $\theta_{\text{min}} = 2.6^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 1999) | $h = -8 \rightarrow 9$ |
| $T_{\text{min}} = 0.960, T_{\text{max}} = 0.966$ | $k = -10 \rightarrow 11$ |
| 8868 measured reflections | $l = -15 \rightarrow 15$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.116$ | $w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.1403P]$ |
| $S = 1.04$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3041 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 186 parameters | $\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$ |
| | Extinction correction: none |

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and

goodness of fit S are based on F^2 , conventional R -factors R are based

on F , with F set to zero for negative F^2 . The threshold expression of

$F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is

not relevant to the choice of reflections for refinement. R -factors based

on F^2 are statistically about twice as large as those based on F , and R -

factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| C1 | -0.38800 (18) | 0.42099 (15) | 0.12980 (11) | 0.0357 (3) |
| C2 | -0.49675 (19) | 0.45875 (16) | 0.20631 (12) | 0.0413 (3) |
| H2 | -0.4480 | 0.5584 | 0.2610 | 0.050* |
| C3 | -0.6764 (2) | 0.34969 (18) | 0.20189 (13) | 0.0469 (3) |
| H3 | -0.7484 | 0.3771 | 0.2527 | 0.056* |
| C4 | -0.7491 (2) | 0.20056 (18) | 0.12250 (14) | 0.0499 (3) |
| H4 | -0.8689 | 0.1265 | 0.1205 | 0.060* |
| C5 | -0.6433 (2) | 0.16181 (18) | 0.04615 (13) | 0.0526 (4) |
| H5 | -0.6916 | 0.0606 | -0.0069 | 0.063* |
| C6 | -0.4668 (2) | 0.27146 (17) | 0.04756 (12) | 0.0448 (3) |
| H6 | -0.3995 | 0.2458 | -0.0066 | 0.054* |
| C7 | -0.19833 (18) | 0.53387 (16) | 0.12988 (12) | 0.0384 (3) |
| C8 | -0.04981 (18) | 0.62292 (15) | 0.22311 (11) | 0.0366 (3) |
| C9 | 0.12813 (18) | 0.73207 (16) | 0.20106 (11) | 0.0375 (3) |
| C10 | 0.47891 (18) | 0.89529 (15) | 0.29540 (11) | 0.0370 (3) |
| H10 | 0.4781 | 0.9476 | 0.2294 | 0.044* |
| C11 | 0.64996 (18) | 0.92856 (15) | 0.38626 (11) | 0.0390 (3) |
| C12 | 0.65136 (19) | 0.84577 (17) | 0.48305 (12) | 0.0439 (3) |
| H12 | 0.7679 | 0.8659 | 0.5429 | 0.053* |
| C13 | 0.4833 (2) | 0.73495 (18) | 0.49135 (12) | 0.0439 (3) |

supplementary materials

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|------|---------------|--------------|--------------|------------|
| H13 | 0.4862 | 0.6800 | 0.5562 | 0.053* |
| C14 | -0.03927 (19) | 0.62083 (18) | 0.35174 (11) | 0.0427 (3) |
| H14A | -0.0509 | 0.7271 | 0.3874 | 0.051* |
| H14B | -0.1486 | 0.5319 | 0.3584 | 0.051* |
| C15 | 0.30664 (17) | 0.78222 (14) | 0.30322 (10) | 0.0336 (3) |
| C16 | 0.30814 (18) | 0.70497 (15) | 0.40210 (11) | 0.0362 (3) |
| C17 | 0.8268 (3) | 1.1358 (3) | 0.29888 (18) | 0.0764 (6) |
| H17A | 0.8124 | 1.0644 | 0.2261 | 0.115* |
| H17B | 0.9493 | 1.2225 | 0.3186 | 0.115* |
| H17C | 0.7195 | 1.1861 | 0.2896 | 0.115* |
| O1 | 0.13097 (14) | 0.77364 (14) | 0.10531 (9) | 0.0566 (3) |
| O2 | 0.14409 (13) | 0.59397 (12) | 0.41471 (8) | 0.0454 (2) |
| O3 | 0.82540 (14) | 1.03993 (13) | 0.38987 (9) | 0.0540 (3) |
| H7 | -0.175 (2) | 0.5435 (19) | 0.0546 (15) | 0.051 (4)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|-------------|-------------|-------------|-------------|-------------|
| C1 | 0.0311 (6) | 0.0373 (6) | 0.0357 (6) | 0.0073 (5) | 0.0046 (5) | 0.0092 (5) |
| C2 | 0.0344 (6) | 0.0382 (6) | 0.0475 (7) | 0.0079 (5) | 0.0088 (5) | 0.0016 (5) |
| C3 | 0.0365 (7) | 0.0516 (8) | 0.0538 (8) | 0.0108 (6) | 0.0158 (6) | 0.0100 (6) |
| C4 | 0.0349 (7) | 0.0470 (7) | 0.0587 (9) | -0.0018 (6) | 0.0082 (6) | 0.0122 (6) |
| C5 | 0.0497 (8) | 0.0431 (7) | 0.0504 (8) | -0.0009 (6) | 0.0048 (6) | -0.0030 (6) |
| C6 | 0.0426 (7) | 0.0480 (7) | 0.0384 (7) | 0.0072 (6) | 0.0091 (5) | 0.0016 (5) |
| C7 | 0.0339 (6) | 0.0423 (6) | 0.0378 (6) | 0.0081 (5) | 0.0092 (5) | 0.0087 (5) |
| C8 | 0.0310 (6) | 0.0403 (6) | 0.0380 (6) | 0.0084 (5) | 0.0097 (5) | 0.0074 (5) |
| C9 | 0.0321 (6) | 0.0423 (6) | 0.0353 (6) | 0.0069 (5) | 0.0071 (5) | 0.0079 (5) |
| C10 | 0.0331 (6) | 0.0381 (6) | 0.0375 (6) | 0.0086 (5) | 0.0064 (5) | 0.0066 (5) |
| C11 | 0.0297 (6) | 0.0386 (6) | 0.0444 (7) | 0.0081 (5) | 0.0059 (5) | 0.0025 (5) |
| C12 | 0.0347 (7) | 0.0539 (8) | 0.0385 (7) | 0.0150 (6) | 0.0006 (5) | 0.0039 (6) |
| C13 | 0.0413 (7) | 0.0551 (8) | 0.0352 (6) | 0.0154 (6) | 0.0067 (5) | 0.0111 (5) |
| C14 | 0.0321 (6) | 0.0548 (8) | 0.0392 (7) | 0.0076 (6) | 0.0114 (5) | 0.0059 (6) |
| C15 | 0.0298 (6) | 0.0357 (6) | 0.0334 (6) | 0.0087 (5) | 0.0067 (5) | 0.0032 (4) |
| C16 | 0.0334 (6) | 0.0401 (6) | 0.0349 (6) | 0.0101 (5) | 0.0100 (5) | 0.0047 (5) |
| C17 | 0.0437 (9) | 0.0871 (13) | 0.0821 (13) | -0.0091 (9) | 0.0049 (8) | 0.0372 (10) |
| O1 | 0.0392 (5) | 0.0764 (7) | 0.0416 (5) | -0.0049 (5) | 0.0035 (4) | 0.0223 (5) |
| O2 | 0.0369 (5) | 0.0580 (6) | 0.0403 (5) | 0.0077 (4) | 0.0104 (4) | 0.0173 (4) |
| O3 | 0.0305 (5) | 0.0574 (6) | 0.0614 (6) | -0.0006 (4) | -0.0003 (4) | 0.0152 (5) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------|-------------|---------|-------------|
| C1—C2 | 1.3932 (18) | C10—C11 | 1.3805 (17) |
| C1—C6 | 1.3978 (17) | C10—C15 | 1.4007 (17) |
| C1—C7 | 1.4671 (17) | C10—H10 | 0.9300 |
| C2—C3 | 1.3830 (19) | C11—O3 | 1.3704 (15) |
| C2—H2 | 0.9300 | C11—C12 | 1.3927 (19) |
| C3—C4 | 1.378 (2) | C12—C13 | 1.371 (2) |
| C3—H3 | 0.9300 | C12—H12 | 0.9300 |
| C4—C5 | 1.377 (2) | C13—C16 | 1.3938 (17) |

| | | | |
|-------------|-------------|-----------------|--------------|
| C4—H4 | 0.9300 | C13—H13 | 0.9300 |
| C5—C6 | 1.377 (2) | C14—O2 | 1.4434 (16) |
| C5—H5 | 0.9300 | C14—H14A | 0.9700 |
| C6—H6 | 0.9300 | C14—H14B | 0.9700 |
| C7—C8 | 1.3412 (17) | C15—C16 | 1.3883 (17) |
| C7—H7 | 0.950 (16) | C16—O2 | 1.3693 (15) |
| C8—C9 | 1.4846 (18) | C17—O3 | 1.403 (2) |
| C8—C14 | 1.5036 (18) | C17—H17A | 0.9600 |
| C9—O1 | 1.2187 (15) | C17—H17B | 0.9600 |
| C9—C15 | 1.4818 (16) | C17—H17C | 0.9600 |
| C2—C1—C6 | 118.20 (12) | O3—C11—C10 | 124.75 (12) |
| C2—C1—C7 | 122.70 (11) | O3—C11—C12 | 115.45 (11) |
| C6—C1—C7 | 119.07 (12) | C10—C11—C12 | 119.80 (12) |
| C3—C2—C1 | 120.72 (12) | C13—C12—C11 | 120.93 (12) |
| C3—C2—H2 | 119.6 | C13—C12—H12 | 119.5 |
| C1—C2—H2 | 119.6 | C11—C12—H12 | 119.5 |
| C4—C3—C2 | 120.26 (13) | C12—C13—C16 | 119.70 (12) |
| C4—C3—H3 | 119.9 | C12—C13—H13 | 120.1 |
| C2—C3—H3 | 119.9 | C16—C13—H13 | 120.1 |
| C5—C4—C3 | 119.63 (13) | O2—C14—C8 | 111.15 (10) |
| C5—C4—H4 | 120.2 | O2—C14—H14A | 109.4 |
| C3—C4—H4 | 120.2 | C8—C14—H14A | 109.4 |
| C6—C5—C4 | 120.64 (13) | O2—C14—H14B | 109.4 |
| C6—C5—H5 | 119.7 | C8—C14—H14B | 109.4 |
| C4—C5—H5 | 119.7 | H14A—C14—H14B | 108.0 |
| C5—C6—C1 | 120.49 (13) | C16—C15—C10 | 120.07 (11) |
| C5—C6—H6 | 119.8 | C16—C15—C9 | 119.69 (11) |
| C1—C6—H6 | 119.8 | C10—C15—C9 | 119.96 (11) |
| C8—C7—C1 | 128.33 (12) | O2—C16—C15 | 122.60 (11) |
| C8—C7—H7 | 115.3 (9) | O2—C16—C13 | 117.53 (11) |
| C1—C7—H7 | 116.4 (9) | C15—C16—C13 | 119.83 (12) |
| C7—C8—C9 | 118.66 (11) | O3—C17—H17A | 109.5 |
| C7—C8—C14 | 126.65 (12) | O3—C17—H17B | 109.5 |
| C9—C8—C14 | 114.65 (10) | H17A—C17—H17B | 109.5 |
| O1—C9—C15 | 121.81 (11) | O3—C17—H17C | 109.5 |
| O1—C9—C8 | 123.09 (11) | H17A—C17—H17C | 109.5 |
| C15—C9—C8 | 115.06 (11) | H17B—C17—H17C | 109.5 |
| C11—C10—C15 | 119.58 (12) | C16—O2—C14 | 113.85 (10) |
| C11—C10—H10 | 120.2 | C11—O3—C17 | 117.35 (11) |
| C15—C10—H10 | 120.2 | | |
| C6—C1—C2—C3 | 0.93 (19) | C11—C12—C13—C16 | -0.3 (2) |
| C7—C1—C2—C3 | 179.01 (12) | C7—C8—C14—O2 | 129.37 (13) |
| C1—C2—C3—C4 | 0.9 (2) | C9—C8—C14—O2 | -48.50 (15) |
| C2—C3—C4—C5 | -1.0 (2) | C11—C10—C15—C16 | 0.33 (18) |
| C3—C4—C5—C6 | -0.7 (2) | C11—C10—C15—C9 | -173.63 (11) |
| C4—C5—C6—C1 | 2.6 (2) | O1—C9—C15—C16 | -166.84 (12) |
| C2—C1—C6—C5 | -2.7 (2) | C8—C9—C15—C16 | 10.83 (17) |
| C7—C1—C6—C5 | 179.18 (12) | O1—C9—C15—C10 | 7.14 (19) |

supplementary materials

| | | | |
|-----------------|--------------|-----------------|--------------|
| C2—C1—C7—C8 | 41.2 (2) | C8—C9—C15—C10 | -175.19 (10) |
| C6—C1—C7—C8 | -140.74 (14) | C10—C15—C16—O2 | 179.75 (11) |
| C1—C7—C8—C9 | -178.86 (12) | C9—C15—C16—O2 | -6.28 (18) |
| C1—C7—C8—C14 | 3.3 (2) | C10—C15—C16—C13 | -2.59 (18) |
| C7—C8—C9—O1 | 16.3 (2) | C9—C15—C16—C13 | 171.39 (11) |
| C14—C8—C9—O1 | -165.66 (13) | C12—C13—C16—O2 | -179.65 (11) |
| C7—C8—C9—C15 | -161.35 (11) | C12—C13—C16—C15 | 2.57 (19) |
| C14—C8—C9—C15 | 16.71 (16) | C15—C16—O2—C14 | -27.22 (16) |
| C15—C10—C11—O3 | -178.13 (11) | C13—C16—O2—C14 | 155.06 (11) |
| C15—C10—C11—C12 | 1.94 (18) | C8—C14—O2—C16 | 53.73 (14) |
| O3—C11—C12—C13 | 178.09 (12) | C10—C11—O3—C17 | 5.0 (2) |
| C10—C11—C12—C13 | -2.0 (2) | C12—C11—O3—C17 | -175.11 (15) |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------|-------|-------------|-------------|---------------|
| C6—H6 \cdots O1 ⁱ | 0.93 | 2.53 | 3.4293 (18) | 163 |

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

Fig. 1

