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# 2-Methoxy-4-(prop-2-en-1-yl)phenyl benzoate

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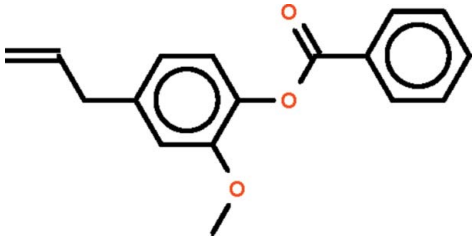
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.051; $wR$ factor = 0.138; data-to-parameter ratio = 17.5.

In the title compound, $C_{17}H_{16}O_3$, the benzene rings are twisted by 63.54 (5)°. The twist is similar to that found in the unsubstituted compound, phenyl benzoate. The crystal packing features C—H···O hydrogen bonds.

## Related literature

For the structure of phenyl benzoate, see: Shibakami & Sekiya (1995).



## Experimental

### Crystal data

$C_{17}H_{16}O_3$
$M_r$ = 268.30
Monoclinic, $P2_1/c$
$a$ = 9.9334 (6) Å
$b$ = 9.5124 (5) Å
$c$ = 14.9463 (9) Å
$\beta$ = 103.405 (6)°
$V$ = 1373.81 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 100 K
0.40 × 0.30 × 0.20 mm

### Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min}$ = 0.966, $T_{max}$ = 0.983
7024 measured reflections
3168 independent reflections
2242 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.138
$S$ = 1.05
3168 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2···O3$^{i}$ | 0.95 | 2.55 | 3.256 (2) | 131 |
| C15—H15···O3$^{ii}$ | 0.95 | 2.54 | 3.209 (2) | 128 |

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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: BT6914).

## References

Agilent (2013). *CrysAlis PRO*. Agilent Technologies Inc., Santa Clara, CA, USA.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shibakami, M. & Sekiya, A. (1995). *Acta Cryst.* C**51**, 326–330.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

*Acta Cryst.* (2013). E**69**, o1088 [https://doi.org/10.1107/S1600536813015791]

## 2-Methoxy-4-(prop-2-en-1-yl)phenyl benzoate

**Mallikarjuna Rao Pichika, Yew Beng Kang and Seik Weng Ng**

### S1. Comment

The title phenyl benzoate (Scheme I, Fig. 1), which possesses an allyl and a methoxy substituent, was synthesized for an evaluation of its pharmaceutical properties as it is an ester derivative of eugenol. The two benzene rings are approximately perpendicular [dihedral angle 63.54 (5)°]. The twist is similar to that found in the unsubstituted compound, phenyl benzoate (Shibakami & Sekiya, 1995).

### S2. Experimental

4-Allyl-2-methoxyphenol (1 mmol), benzoic acid (1 mmol), diethylazodicarboxylate (2 mmol) and triphenylphosphine (2 mmol) were heated in THF (10 ml) for 2 h. The solid material extracted with dichloromethane. The dichloromethane solution was eluted through a silica gel column by using an *n*-hexane–ethyl acetate (95: 5 *v*/*v*) solvent system. Slow evaporation of the solution yielded large colorless crystals.

### S3. Refinement

H-atoms were placed in calculated positions [C–H 0.95 to 0.98 Å, $U_{iso}$(H) 1.2 to 1.5$U_{eq}$(C)] and were included in the refinement in the riding model approximation.

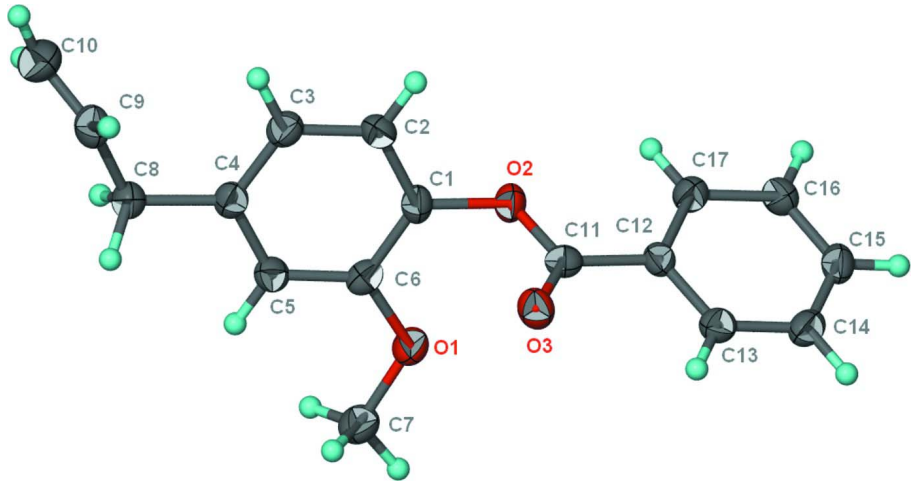


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $C_{17}H_{16}O_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## 2-Methoxy-4-(prop-2-en-1-yl)phenyl benzoate

*Crystal data*

$C_{17}H_{16}O_3$
$M_r = 268.30$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.9334$ (6) Å
$b = 9.5124$ (5) Å
$c = 14.9463$ (9) Å
$\beta = 103.405$ (6)°
$V = 1373.81$ (14) Å$^3$
$Z = 4$
$F(000) = 568$
$D_x = 1.297$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1957 reflections
$\theta = 3.0$–$27.5°$
$\mu = 0.09$ mm$^{-1}$
$T = 100$ K
Prism, colorless
0.40 × 0.30 × 0.20 mm

*Data collection*

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min} = 0.966$, $T_{max} = 0.983$
7024 measured reflections
3168 independent reflections
2242 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.0°$
$h = -10 \rightarrow 12$
$k = -9 \rightarrow 12$
$l = -19 \rightarrow 16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.138$
$S = 1.05$
3168 reflections
181 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.1625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.40190 (12) | 0.28310 (12) | 0.60263 (8) | 0.0266 (3) |
| O2 | 0.22747 (12) | 0.48286 (12) | 0.63406 (8) | 0.0241 (3) |
| O3 | 0.09998 (13) | 0.28409 (12) | 0.60909 (8) | 0.0266 (3) |
| C1 | 0.25534 (17) | 0.47175 (17) | 0.54614 (11) | 0.0216 (4) |
| C2 | 0.19517 (17) | 0.56488 (17) | 0.47895 (12) | 0.0232 (4) |
| H2 | 0.1302 | 0.6319 | 0.4904 | 0.028* |
| C3 | 0.22950 (17) | 0.56121 (18) | 0.39346 (12) | 0.0236 (4) |
| H3 | 0.1877 | 0.6257 | 0.3467 | 0.028* |
| C4 | 0.32409 (17) | 0.46399 (17) | 0.37666 (11) | 0.0216 (4) |
| C5 | 0.38323 (17) | 0.36863 (17) | 0.44573 (11) | 0.0220 (4) |
| H5 | 0.4472 | 0.3007 | 0.4341 | 0.026* |
| C6 | 0.35012 (17) | 0.37154 (17) | 0.53098 (11) | 0.0218 (4) |
| C7 | 0.48978 (19) | 0.1729 (2) | 0.58544 (13) | 0.0305 (4) |

| | | | | |
|---|---|---|---|---|
| H7A | 0.5215 | 0.1171 | 0.6415 | 0.046* |
| H7B | 0.5699 | 0.2133 | 0.5669 | 0.046* |
| H7C | 0.4384 | 0.1124 | 0.5361 | 0.046* |
| C8 | 0.36682 (18) | 0.45729 (18) | 0.28547 (11) | 0.0241 (4) |
| H8A | 0.4647 | 0.4870 | 0.2957 | 0.029* |
| H8B | 0.3613 | 0.3583 | 0.2645 | 0.029* |
| C9 | 0.2825 (2) | 0.5455 (2) | 0.21071 (12) | 0.0300 (4) |
| H9 | 0.1877 | 0.5214 | 0.1888 | 0.036* |
| C10 | 0.3292 (3) | 0.6537 (2) | 0.17302 (14) | 0.0429 (5) |
| H10A | 0.4234 | 0.6809 | 0.1931 | 0.052* |
| H10B | 0.2690 | 0.7049 | 0.1255 | 0.052* |
| C11 | 0.15078 (17) | 0.37820 (17) | 0.65969 (12) | 0.0215 (4) |
| C12 | 0.13802 (17) | 0.39478 (17) | 0.75630 (11) | 0.0206 (4) |
| C13 | 0.08089 (17) | 0.28421 (18) | 0.79540 (12) | 0.0233 (4) |
| H13 | 0.0493 | 0.2026 | 0.7601 | 0.028* |
| C14 | 0.06989 (18) | 0.29291 (19) | 0.88614 (12) | 0.0264 (4) |
| H14 | 0.0324 | 0.2164 | 0.9133 | 0.032* |
| C15 | 0.11346 (18) | 0.41292 (18) | 0.93709 (12) | 0.0261 (4) |
| H15 | 0.1064 | 0.4185 | 0.9993 | 0.031* |
| C16 | 0.16721 (18) | 0.52473 (18) | 0.89742 (12) | 0.0262 (4) |
| H16 | 0.1947 | 0.6079 | 0.9320 | 0.031* |
| C17 | 0.18109 (18) | 0.51586 (18) | 0.80734 (12) | 0.0233 (4) |
| H17 | 0.2198 | 0.5920 | 0.7806 | 0.028* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0297 (7) | 0.0284 (7) | 0.0225 (6) | 0.0055 (6) | 0.0076 (5) | 0.0056 (5) |
| O2 | 0.0305 (7) | 0.0244 (6) | 0.0196 (6) | −0.0024 (5) | 0.0102 (5) | −0.0015 (5) |
| O3 | 0.0295 (7) | 0.0267 (7) | 0.0244 (7) | −0.0031 (6) | 0.0082 (5) | −0.0049 (5) |
| C1 | 0.0244 (9) | 0.0236 (9) | 0.0183 (8) | −0.0042 (7) | 0.0078 (7) | −0.0027 (7) |
| C2 | 0.0261 (9) | 0.0196 (8) | 0.0255 (9) | 0.0013 (7) | 0.0089 (7) | −0.0018 (7) |
| C3 | 0.0268 (9) | 0.0228 (8) | 0.0210 (9) | −0.0002 (8) | 0.0048 (7) | 0.0019 (7) |
| C4 | 0.0247 (9) | 0.0211 (8) | 0.0193 (8) | −0.0039 (7) | 0.0054 (7) | −0.0022 (7) |
| C5 | 0.0208 (9) | 0.0215 (8) | 0.0251 (9) | 0.0002 (7) | 0.0079 (7) | 0.0000 (7) |
| C6 | 0.0219 (8) | 0.0215 (8) | 0.0212 (8) | −0.0028 (7) | 0.0032 (7) | 0.0027 (7) |
| C7 | 0.0315 (10) | 0.0299 (10) | 0.0310 (10) | 0.0054 (9) | 0.0094 (8) | 0.0073 (8) |
| C8 | 0.0283 (9) | 0.0243 (9) | 0.0210 (9) | 0.0010 (8) | 0.0081 (7) | 0.0000 (7) |
| C9 | 0.0360 (10) | 0.0338 (10) | 0.0212 (9) | 0.0042 (9) | 0.0087 (8) | −0.0002 (8) |
| C10 | 0.0651 (15) | 0.0344 (11) | 0.0321 (11) | 0.0090 (11) | 0.0171 (11) | 0.0076 (9) |
| C11 | 0.0210 (8) | 0.0197 (8) | 0.0232 (9) | 0.0028 (7) | 0.0039 (7) | 0.0016 (7) |
| C12 | 0.0214 (8) | 0.0223 (8) | 0.0189 (8) | 0.0045 (7) | 0.0060 (6) | 0.0010 (7) |
| C13 | 0.0230 (9) | 0.0218 (9) | 0.0255 (9) | 0.0016 (7) | 0.0066 (7) | 0.0010 (7) |
| C14 | 0.0263 (9) | 0.0260 (9) | 0.0291 (10) | 0.0026 (8) | 0.0109 (7) | 0.0070 (8) |
| C15 | 0.0285 (9) | 0.0315 (10) | 0.0199 (9) | 0.0070 (8) | 0.0087 (7) | 0.0033 (8) |
| C16 | 0.0319 (10) | 0.0243 (9) | 0.0232 (9) | 0.0011 (8) | 0.0079 (8) | −0.0030 (7) |
| C17 | 0.0254 (9) | 0.0221 (9) | 0.0230 (9) | −0.0012 (7) | 0.0068 (7) | 0.0008 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C6 | 1.3652 (19) | C8—H8A | 0.9900 |
| O1—C7 | 1.425 (2) | C8—H8B | 0.9900 |
| O2—C11 | 1.361 (2) | C9—C10 | 1.309 (3) |
| O2—C1 | 1.4084 (19) | C9—H9 | 0.9500 |
| O3—C11 | 1.205 (2) | C10—H10A | 0.9500 |
| C1—C2 | 1.368 (2) | C10—H10B | 0.9500 |
| C1—C6 | 1.395 (2) | C11—C12 | 1.487 (2) |
| C2—C3 | 1.397 (2) | C12—C13 | 1.387 (2) |
| C2—H2 | 0.9500 | C12—C17 | 1.393 (2) |
| C3—C4 | 1.382 (2) | C13—C14 | 1.388 (2) |
| C3—H3 | 0.9500 | C13—H13 | 0.9500 |
| C4—C5 | 1.397 (2) | C14—C15 | 1.385 (2) |
| C4—C8 | 1.520 (2) | C14—H14 | 0.9500 |
| C5—C6 | 1.388 (2) | C15—C16 | 1.384 (2) |
| C5—H5 | 0.9500 | C15—H15 | 0.9500 |
| C7—H7A | 0.9800 | C16—C17 | 1.387 (2) |
| C7—H7B | 0.9800 | C16—H16 | 0.9500 |
| C7—H7C | 0.9800 | C17—H17 | 0.9500 |
| C8—C9 | 1.490 (2) | | |
| | | | |
| C6—O1—C7 | 116.55 (13) | C4—C8—H8B | 108.5 |
| C11—O2—C1 | 116.84 (13) | H8A—C8—H8B | 107.5 |
| C2—C1—C6 | 121.32 (15) | C10—C9—C8 | 124.85 (19) |
| C2—C1—O2 | 119.29 (15) | C10—C9—H9 | 117.6 |
| C6—C1—O2 | 119.27 (14) | C8—C9—H9 | 117.6 |
| C1—C2—C3 | 119.82 (16) | C9—C10—H10A | 120.0 |
| C1—C2—H2 | 120.1 | C9—C10—H10B | 120.0 |
| C3—C2—H2 | 120.1 | H10A—C10—H10B | 120.0 |
| C4—C3—C2 | 120.21 (16) | O3—C11—O2 | 123.18 (15) |
| C4—C3—H3 | 119.9 | O3—C11—C12 | 124.81 (16) |
| C2—C3—H3 | 119.9 | O2—C11—C12 | 112.02 (14) |
| C3—C4—C5 | 119.15 (15) | C13—C12—C17 | 120.00 (15) |
| C3—C4—C8 | 122.27 (15) | C13—C12—C11 | 117.65 (15) |
| C5—C4—C8 | 118.58 (15) | C17—C12—C11 | 122.34 (15) |
| C6—C5—C4 | 121.12 (16) | C12—C13—C14 | 119.94 (16) |
| C6—C5—H5 | 119.4 | C12—C13—H13 | 120.0 |
| C4—C5—H5 | 119.4 | C14—C13—H13 | 120.0 |
| O1—C6—C5 | 125.55 (15) | C15—C14—C13 | 120.07 (16) |
| O1—C6—C1 | 116.07 (14) | C15—C14—H14 | 120.0 |
| C5—C6—C1 | 118.37 (15) | C13—C14—H14 | 120.0 |
| O1—C7—H7A | 109.5 | C16—C15—C14 | 120.03 (16) |
| O1—C7—H7B | 109.5 | C16—C15—H15 | 120.0 |
| H7A—C7—H7B | 109.5 | C14—C15—H15 | 120.0 |
| O1—C7—H7C | 109.5 | C15—C16—C17 | 120.27 (16) |
| H7A—C7—H7C | 109.5 | C15—C16—H16 | 119.9 |
| H7B—C7—H7C | 109.5 | C17—C16—H16 | 119.9 |

| | | | |
|---|---|---|---|
| C9—C8—C4 | 115.06 (14) | C16—C17—C12 | 119.65 (16) |
| C9—C8—H8A | 108.5 | C16—C17—H17 | 120.2 |
| C4—C8—H8A | 108.5 | C12—C17—H17 | 120.2 |
| C9—C8—H8B | 108.5 | | |
| | | | |
| C11—O2—C1—C2 | 111.20 (17) | C3—C4—C8—C9 | −10.0 (2) |
| C11—O2—C1—C6 | −72.7 (2) | C5—C4—C8—C9 | 170.21 (15) |
| C6—C1—C2—C3 | −0.5 (3) | C4—C8—C9—C10 | 114.8 (2) |
| O2—C1—C2—C3 | 175.52 (14) | C1—O2—C11—O3 | −4.8 (2) |
| C1—C2—C3—C4 | −0.1 (3) | C1—O2—C11—C12 | 175.22 (13) |
| C2—C3—C4—C5 | 0.8 (2) | O3—C11—C12—C13 | 9.7 (2) |
| C2—C3—C4—C8 | −178.92 (15) | O2—C11—C12—C13 | −170.29 (14) |
| C3—C4—C5—C6 | −1.0 (2) | O3—C11—C12—C17 | −170.28 (16) |
| C8—C4—C5—C6 | 178.77 (15) | O2—C11—C12—C17 | 9.7 (2) |
| C7—O1—C6—C5 | −4.6 (2) | C17—C12—C13—C14 | −1.6 (3) |
| C7—O1—C6—C1 | 174.89 (15) | C11—C12—C13—C14 | 178.36 (15) |
| C4—C5—C6—O1 | 179.88 (15) | C12—C13—C14—C15 | 1.2 (3) |
| C4—C5—C6—C1 | 0.4 (2) | C13—C14—C15—C16 | 0.4 (3) |
| C2—C1—C6—O1 | −179.15 (15) | C14—C15—C16—C17 | −1.7 (3) |
| O2—C1—C6—O1 | 4.8 (2) | C15—C16—C17—C12 | 1.3 (3) |
| C2—C1—C6—C5 | 0.4 (2) | C13—C12—C17—C16 | 0.4 (3) |
| O2—C1—C6—C5 | −175.68 (14) | C11—C12—C17—C16 | −179.62 (15) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O3$^{i}$ | 0.95 | 2.55 | 3.256 (2) | 131 |
| C15—H15···O3$^{ii}$ | 0.95 | 2.54 | 3.209 (2) | 128 |

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2.