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Ethyl 6-methoxy-2-naphthoate

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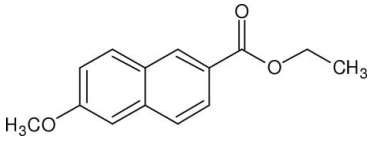
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.103; data-to-parameter ratio = 14.4.

The title compound, $C_{14}H_{14}O_3$, is a starting compound for the synthesis of non-steroidal anti-inflammatory drugs and is an important substrate in the pharmaceutical industry. Whereas the methoxy group is almost coplanar with the naphthyl ring system, the ethoxy group is significantly twisted out of the plane of the aromatic system [C—O—C—C = −85.31 (15)°].

Related literature

Some related crystal structures such as methyl 7-methoxy-2-naphthoate (Prince *et al.*, 1991), 2-acetylphenyl 1-naphthoate (Goeta *et al.*, 1996), methyl 1-hydroxy-2-naphthoate (Jin & Xiao, 2005), ethyl 3-hydroxy-2-naphthoate (Jin & Jin, 2005) and ethyl 4-acetoxy-6-(dimethylamino)-2-naphthoate (Du *et al.*, 2006) have been reported.



Experimental

Crystal data

$C_{14}H_{14}O_3$
M_r = 230.25
Orthorhombic, *Pbca*
a = 14.7132 (9) Å
b = 6.1977 (4) Å
c = 25.362 (2) Å
V = 2312.7 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
0.23 × 0.22 × 0.08 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
16684 measured reflections
2256 independent reflections
1767 reflections with $I > 2\sigma(I)$
R_{int} = 0.080

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.01
2256 reflections
157 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

SB thanks Strides Arco Labs, Mangalore, for a gift sample of the title compound.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2368).

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  doi:10.1107/S1600536807017977

supplementary materials

Acta Cryst. (2007). E**63**, o2350 [**doi:10.1107/S1600536807017977**]

Ethyl 6-methoxy-2-naphthoate

H. S. Yathirajan, S. Bindya, B. K. Sarojini, B. Narayana and M. Bolte

Experimental

A sample of ethyl 6-methoxy-2-naphthoate was obtained from Strides Arco Labs, Mangalore, India. Colourless plates of (I) were obtained by slow evaporation using a mixture (1:1 v/v) of acetone and toluene (m.p.: 359-361 K).

Refinement

The H atoms were found in a difference map, relocated in idelised loations (C—H = 0.95-0.99 Å), and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C_{methyl}). The methyl groups were allowed to rotate but not to tip.

Figures

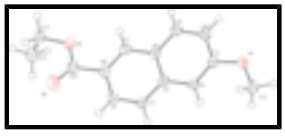

Fig. 1. Perspective view of (I) with displacement ellipsoids shown at the 50% probability level (arbitrary spheres for the H atoms).

Ethyl 6-methoxy-2-naphthoate

Crystal data

$C_{14}H_{14}O_3$	F_{000} = 976
M_r = 230.25	D_x = 1.323 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 12140 reflections
a = 14.7132 (9) Å	θ = 2.8–26.2º
b = 6.1977 (4) Å	μ = 0.09 mm^{-1}
c = 25.362 (2) Å	*T* = 173 (2) K
V = 2312.7 (3) Å^3	Plate, colourless
Z = 8	0.23 × 0.22 × 0.08 mm

Data collection

Stoe IPDSII two-circle diffractometer	1767 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.080
Monochromator: graphite	θ_{max} = 26.0º
T = 173(2) K	θ_{min} = 2.8º
ω scans	*h* = −18→18

Absorption correction: none
16684 measured reflections
2256 independent reflections

$k = -7 \rightarrow 7$
$l = -31 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.103$

$S = 1.01$

2256 reflections

157 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.24$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.013 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.36698 (6)	0.29857 (16)	0.09601 (4)	0.0312 (3)
O2	0.39644 (8)	0.39529 (18)	0.43943 (4)	0.0477 (3)
O3	0.41704 (7)	0.72652 (16)	0.40506 (4)	0.0347 (3)
C1	0.37321 (8)	0.3496 (2)	0.14820 (5)	0.0249 (3)
C2	0.34544 (7)	0.2212 (2)	0.18942 (5)	0.0236 (3)
H2	0.3187	0.0844	0.1827	0.028*
C3	0.35702 (7)	0.2947 (2)	0.24217 (5)	0.0222 (3)
C4	0.33292 (8)	0.1654 (2)	0.28634 (5)	0.0254 (3)
H4	0.3067	0.0273	0.2808	0.031*
C5	0.34697 (8)	0.2369 (2)	0.33686 (5)	0.0268 (3)
H5	0.3317	0.1466	0.3658	0.032*
C6	0.38419 (8)	0.4450 (2)	0.34625 (5)	0.0260 (3)

C7	0.40703 (7)	0.5744 (2)	0.30413 (5)	0.0242 (3)
H7	0.4312	0.7141	0.3104	0.029*
C8	0.39510 (7)	0.5030 (2)	0.25179 (5)	0.0224 (3)
C9	0.42163 (8)	0.6307 (2)	0.20785 (5)	0.0270 (3)
H9	0.4464	0.7703	0.2135	0.032*
C10	0.41193 (8)	0.5553 (2)	0.15761 (5)	0.0279 (3)
H10	0.4313	0.6414	0.1287	0.033*
C11	0.34036 (11)	0.0852 (3)	0.08202 (6)	0.0402 (4)
H11A	0.3807	−0.0189	0.0993	0.060*
H11B	0.3444	0.0676	0.0437	0.060*
H11C	0.2776	0.0600	0.0934	0.060*
C12	0.39926 (8)	0.5145 (2)	0.40172 (5)	0.0293 (3)
C13	0.43231 (10)	0.8154 (3)	0.45740 (6)	0.0374 (4)
H13A	0.4711	0.9455	0.4547	0.045*
H13B	0.4647	0.7080	0.4794	0.045*
C14	0.34401 (10)	0.8739 (3)	0.48323 (6)	0.0396 (4)
H14A	0.3104	0.9738	0.4605	0.059*
H14B	0.3561	0.9431	0.5173	0.059*
H14C	0.3079	0.7431	0.4888	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0391 (5)	0.0326 (6)	0.0220 (5)	−0.0022 (4)	−0.0029 (4)	0.0000 (4)
O2	0.0764 (8)	0.0391 (6)	0.0276 (6)	0.0000 (5)	−0.0048 (5)	0.0013 (5)
O3	0.0443 (6)	0.0352 (6)	0.0247 (5)	−0.0072 (4)	0.0025 (4)	−0.0087 (4)
C1	0.0245 (6)	0.0281 (7)	0.0221 (7)	0.0031 (5)	−0.0026 (5)	0.0001 (5)
C2	0.0234 (5)	0.0214 (6)	0.0260 (7)	−0.0012 (5)	−0.0025 (5)	−0.0003 (5)
C3	0.0183 (5)	0.0223 (7)	0.0259 (7)	0.0015 (5)	−0.0013 (4)	0.0003 (5)
C4	0.0259 (6)	0.0230 (7)	0.0274 (7)	−0.0031 (5)	−0.0004 (5)	0.0006 (5)
C5	0.0292 (6)	0.0266 (7)	0.0245 (7)	−0.0007 (5)	0.0013 (5)	0.0036 (5)
C6	0.0232 (6)	0.0295 (7)	0.0251 (7)	0.0034 (5)	0.0001 (5)	−0.0028 (5)
C7	0.0226 (6)	0.0212 (6)	0.0290 (7)	0.0004 (5)	−0.0009 (5)	−0.0019 (5)
C8	0.0189 (5)	0.0215 (7)	0.0267 (7)	0.0013 (5)	−0.0008 (4)	−0.0003 (5)
C9	0.0277 (6)	0.0219 (6)	0.0313 (8)	−0.0026 (5)	−0.0007 (5)	0.0024 (5)
C10	0.0305 (6)	0.0267 (7)	0.0264 (7)	−0.0010 (5)	0.0010 (5)	0.0058 (5)
C11	0.0552 (9)	0.0368 (9)	0.0284 (8)	−0.0070 (7)	−0.0050 (6)	−0.0053 (6)
C12	0.0288 (6)	0.0321 (7)	0.0269 (7)	0.0018 (5)	0.0013 (5)	−0.0022 (6)
C13	0.0407 (7)	0.0443 (9)	0.0271 (8)	−0.0090 (6)	0.0003 (6)	−0.0123 (6)
C14	0.0456 (8)	0.0403 (9)	0.0329 (8)	−0.0011 (7)	0.0040 (6)	−0.0076 (7)

Geometric parameters (Å, °)

O1—C1	1.3642 (16)	C6—C12	1.4880 (19)
O1—C11	1.4240 (18)	C7—C8	1.4102 (18)
O2—C12	1.2089 (18)	C7—H7	0.9500
O3—C12	1.3427 (17)	C8—C9	1.4216 (18)
O3—C13	1.4547 (17)	C9—C10	1.3646 (19)
C1—C2	1.3758 (18)	C9—H9	0.9500

C1—C10	1.4165 (19)	C10—H10	0.9500
C2—C3	1.4234 (18)	C11—H11A	0.9800
C2—H2	0.9500	C11—H11B	0.9800
C3—C4	1.4219 (18)	C11—H11C	0.9800
C3—C8	1.4284 (17)	C13—C14	1.500 (2)
C4—C5	1.3715 (19)	C13—H13A	0.9900
C4—H4	0.9500	C13—H13B	0.9900
C5—C6	1.4209 (19)	C14—H14A	0.9800
C5—H5	0.9500	C14—H14B	0.9800
C6—C7	1.3776 (18)	C14—H14C	0.9800
C1—O1—C11	118.39 (11)	C10—C9—H9	119.6
C12—O3—C13	117.27 (11)	C8—C9—H9	119.6
O1—C1—C2	125.68 (12)	C9—C10—C1	120.50 (12)
O1—C1—C10	113.52 (11)	C9—C10—H10	119.8
C2—C1—C10	120.80 (12)	C1—C10—H10	119.8
C1—C2—C3	119.57 (11)	O1—C11—H11A	109.5
C1—C2—H2	120.2	O1—C11—H11B	109.5
C3—C2—H2	120.2	H11A—C11—H11B	109.5
C4—C3—C2	122.03 (11)	O1—C11—H11C	109.5
C4—C3—C8	118.18 (11)	H11A—C11—H11C	109.5
C2—C3—C8	119.78 (11)	H11B—C11—H11C	109.5
C5—C4—C3	121.10 (12)	O2—C12—O3	123.70 (13)
C5—C4—H4	119.4	O2—C12—C6	124.46 (13)
C3—C4—H4	119.4	O3—C12—C6	111.83 (12)
C4—C5—C6	120.52 (12)	O3—C13—C14	110.88 (12)
C4—C5—H5	119.7	O3—C13—H13A	109.5
C6—C5—H5	119.7	C14—C13—H13A	109.5
C7—C6—C5	119.50 (12)	O3—C13—H13B	109.5
C7—C6—C12	121.90 (12)	C14—C13—H13B	109.5
C5—C6—C12	118.59 (12)	H13A—C13—H13B	108.1
C6—C7—C8	121.12 (12)	C13—C14—H14A	109.5
C6—C7—H7	119.4	C13—C14—H14B	109.5
C8—C7—H7	119.4	H14A—C14—H14B	109.5
C7—C8—C9	121.94 (11)	C13—C14—H14C	109.5
C7—C8—C3	119.56 (11)	H14A—C14—H14C	109.5
C9—C8—C3	118.49 (11)	H14B—C14—H14C	109.5
C10—C9—C8	120.84 (12)		
C11—O1—C1—C2	−8.42 (18)	C2—C3—C8—C7	−179.56 (10)
C11—O1—C1—C10	171.85 (11)	C4—C3—C8—C9	178.33 (11)
O1—C1—C2—C3	179.35 (11)	C2—C3—C8—C9	−0.81 (16)
C10—C1—C2—C3	−0.94 (17)	C7—C8—C9—C10	177.99 (11)
C1—C2—C3—C4	−177.47 (11)	C3—C8—C9—C10	−0.73 (17)
C1—C2—C3—C8	1.64 (16)	C8—C9—C10—C1	1.45 (18)
C2—C3—C4—C5	178.18 (11)	O1—C1—C10—C9	179.14 (11)
C8—C3—C4—C5	−0.94 (17)	C2—C1—C10—C9	−0.61 (18)
C3—C4—C5—C6	1.47 (18)	C13—O3—C12—O2	−0.89 (19)
C4—C5—C6—C7	−0.62 (18)	C13—O3—C12—C6	179.47 (11)
C4—C5—C6—C12	−179.26 (11)	C7—C6—C12—O2	−165.77 (13)

C5—C6—C7—C8	−0.76 (17)	C5—C6—C12—O2	12.84 (19)
C12—C6—C7—C8	177.83 (11)	C7—C6—C12—O3	13.87 (16)
C6—C7—C8—C9	−177.43 (11)	C5—C6—C12—O3	−167.53 (11)
C6—C7—C8—C3	1.27 (17)	C12—O3—C13—C14	−85.31 (15)
C4—C3—C8—C7	−0.42 (16)		

Fig. 1