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Ethyl (naphthalen-2-yloxy)acetate

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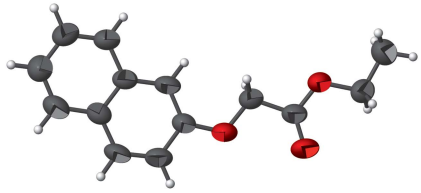
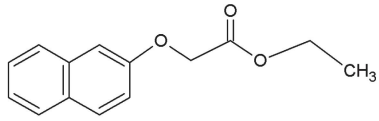
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{14}H_{14}O_3$, the dihedral angle between the naphthyl ring system and the side chain is 9.00 (14)°, and the ethoxy chain adopts an extended conformation [C—O—C—C = 176.0 (3)°]. There are no directional interactions in the crystal beyond normal van der Waals contacts.

3D view



Chemical scheme



Structure description

As part of our interest in intermediates used to prepare naproxen, a non-steroidal anti-inflammatory drug, the synthesis and crystal structure of the title compound is reported here. For related structures, see: Ravikumar *et al.* (1985) and Bond *et al.* (2013).

The dihedral angle between the naphthyl ring system and the side chain is 9.00 (14)° (Fig. 1) and the ethoxy chain adopts an extended conformation [C12—O3—C13—C14 = 176.0 (3)°]. There are no directional interactions in the crystal beyond normal van der Waals contacts. The crystal packing is shown in Fig. 2.

Synthesis and crystallization

2-Naphthol (0.1 mol) was dissolved in 250 ml of dry acetone and mixed with anhydrous potassium carbonate (0.16 mol). Ethyl chloroacetate (0.1 mol) was added and the mixture refluxed for 5–6 h. The progress of the reaction was monitored by thin layer chromatography; upon completion, the reaction mixture was filtered and the solvent removed under reduced pressure. The product obtained was recrystallized from ethanol solution.

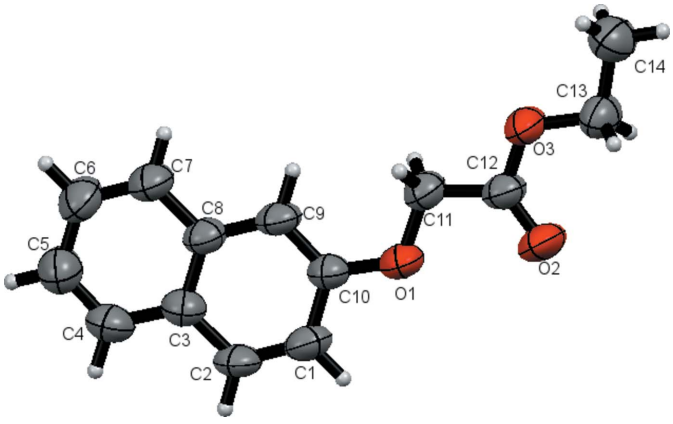


Figure 1
A view of the title molecule, with displacement ellipsoids drawn at the 50% probability level.

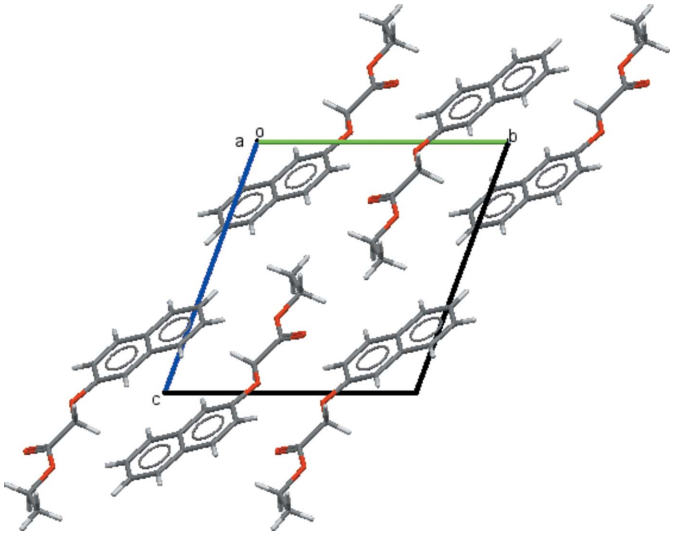


Figure 2
A view along the *a* axis of the crystal packing of the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{14}O_3$
M_r	230.25
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	6.0504 (11), 10.2188 (13), 10.8744 (16)
α, β, γ (°)	106.062 (12), 102.923 (14), 103.358 (14)
V (Å^3)	598.15 (17)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.31 × 0.26 × 0.23
Data collection	
Diffractometer	Rigaku Saturn724+ CCD
Absorption correction	Multi-scan (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.973, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6262, 2265, 1133
R_{int}	0.083
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.083, 0.259, 1.04
No. of reflections	2265
No. of parameters	155
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.21

Computer programs: *CrystalClear SM Expert* (Rigaku, 2011), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *OLEX2* (Dolomanov *et al.*, 2009).

Acknowledgements

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full crystallographic data

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Crystal data

$C_{14}H_{14}O_3$
M_r = 230.25
Triclinic, $P\overline{1}$
a = 6.0504 (11) Å
b = 10.2188 (13) Å
c = 10.8744 (16) Å
α = 106.062 (12)°
β = 102.923 (14)°
γ = 103.358 (14)°
V = 598.15 (17) Å^3
Z = 2
$F(000)$ = 244
D_x = 1.278 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2265 reflections
θ = 2.2–25.7°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.31 × 0.26 × 0.23 mm

Data collection

Rigaku Saturn724+ CCD diffractometer
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku, 1999)
T_{min} = 0.973, T_{max} = 0.980
6262 measured reflections
2265 independent reflections
1133 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 25.7°, θ_{min} = 2.2°
h = −7→7
k = −10→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.259
S = 1.04
2265 reflections
155 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.113P)^2 + 0.0443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.2337 (4)	0.3569 (3)	0.9618 (2)	0.0765 (8)
O2	0.2739 (5)	0.4668 (3)	0.7673 (3)	0.0915 (10)
O3	0.5040 (5)	0.3364 (3)	0.7049 (2)	0.0783 (9)
C1	0.0300 (6)	0.3263 (4)	1.1143 (4)	0.0719 (11)
H1	−0.0336	0.3969	1.0988	0.086*
C2	−0.0308 (6)	0.2642 (4)	1.2017 (4)	0.0755 (11)
H2	−0.1382	0.2915	1.2446	0.091*
C3	0.0669 (6)	0.1581 (4)	1.2292 (4)	0.0692 (10)
C4	0.0083 (7)	0.0897 (4)	1.3181 (4)	0.0823 (12)
H4	−0.1001	0.1136	1.3618	0.099*
C5	0.1070 (8)	−0.0108 (5)	1.3414 (4)	0.0904 (13)
H5	0.0686	−0.0533	1.4025	0.108*
C6	0.2645 (8)	−0.0510 (4)	1.2754 (4)	0.0896 (13)
H6	0.3278	−0.1220	1.2903	0.108*
C7	0.3263 (7)	0.0129 (4)	1.1895 (4)	0.0789 (12)
H7	0.4360	−0.0125	1.1476	0.095*
C8	0.2261 (6)	0.1186 (4)	1.1622 (3)	0.0641 (10)
C9	0.2891 (6)	0.1861 (4)	1.0725 (4)	0.0679 (10)
H9	0.4001	0.1629	1.0307	0.082*
C10	0.1873 (6)	0.2851 (4)	1.0473 (3)	0.0626 (9)
C11	0.3813 (6)	0.3139 (4)	0.8862 (3)	0.0696 (10)
H11A	0.3247	0.2105	0.8429	0.084*
H11B	0.5432	0.3412	0.9450	0.084*
C12	0.3782 (6)	0.3843 (4)	0.7817 (3)	0.0672 (10)
C13	0.5213 (7)	0.3934 (4)	0.5988 (4)	0.0809 (12)
H13A	0.5844	0.4972	0.6355	0.097*
H13B	0.3649	0.3663	0.5341	0.097*
C14	0.6823 (7)	0.3339 (5)	0.5331 (4)	0.1014 (15)
H14A	0.6934	0.3679	0.4600	0.152*
H14B	0.6205	0.2311	0.4992	0.152*
H14C	0.8380	0.3640	0.5972	0.152*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0922 (19)	0.0789 (17)	0.0901 (18)	0.0563 (15)	0.0460 (15)	0.0383 (15)
O2	0.107 (2)	0.108 (2)	0.103 (2)	0.0777 (18)	0.0463 (16)	0.0527 (17)
O3	0.107 (2)	0.0873 (18)	0.0788 (17)	0.0646 (16)	0.0473 (15)	0.0437 (14)
C1	0.070 (2)	0.076 (3)	0.079 (3)	0.044 (2)	0.024 (2)	0.024 (2)
C2	0.079 (3)	0.084 (3)	0.084 (3)	0.051 (2)	0.043 (2)	0.026 (2)
C3	0.076 (2)	0.072 (2)	0.072 (2)	0.035 (2)	0.0347 (19)	0.0232 (19)
C4	0.085 (3)	0.095 (3)	0.086 (3)	0.046 (2)	0.046 (2)	0.030 (2)
C5	0.114 (3)	0.093 (3)	0.089 (3)	0.048 (3)	0.047 (3)	0.044 (2)
C6	0.123 (4)	0.080 (3)	0.094 (3)	0.058 (3)	0.045 (3)	0.042 (3)
C7	0.094 (3)	0.081 (3)	0.087 (3)	0.054 (2)	0.041 (2)	0.035 (2)

C8	0.070 (2)	0.061 (2)	0.069 (2)	0.0342 (19)	0.0258 (18)	0.0198 (18)
C9	0.071 (2)	0.070 (2)	0.078 (2)	0.0433 (19)	0.0319 (19)	0.023 (2)
C10	0.067 (2)	0.066 (2)	0.067 (2)	0.0345 (18)	0.0293 (18)	0.0231 (18)
C11	0.084 (2)	0.069 (2)	0.073 (2)	0.042 (2)	0.0305 (19)	0.0296 (19)
C12	0.069 (2)	0.070 (2)	0.074 (2)	0.039 (2)	0.0261 (18)	0.0254 (19)
C13	0.104 (3)	0.093 (3)	0.069 (2)	0.054 (2)	0.033 (2)	0.039 (2)
C14	0.121 (4)	0.131 (4)	0.092 (3)	0.072 (3)	0.054 (3)	0.055 (3)

Geometric parameters (Å, º)

O1—C10	1.372 (4)	C6—H6	0.9300
O1—C11	1.406 (4)	C6—C7	1.349 (5)
O2—C12	1.187 (4)	C7—H7	0.9300
O3—C12	1.322 (4)	C7—C8	1.421 (5)
O3—C13	1.442 (4)	C8—C9	1.411 (5)
C1—H1	0.9300	C9—H9	0.9300
C1—C2	1.350 (5)	C9—C10	1.358 (5)
C1—C10	1.393 (4)	C11—H11A	0.9700
C2—H2	0.9300	C11—H11B	0.9700
C2—C3	1.418 (5)	C11—C12	1.502 (5)
C3—C4	1.402 (5)	C13—H13A	0.9700
C3—C8	1.397 (5)	C13—H13B	0.9700
C4—H4	0.9300	C13—C14	1.474 (5)
C4—C5	1.355 (5)	C14—H14A	0.9600
C5—H5	0.9300	C14—H14B	0.9600
C5—C6	1.384 (5)	C14—H14C	0.9600
C10—O1—C11	116.5 (2)	C10—C9—C8	119.9 (3)
C12—O3—C13	117.0 (3)	C10—C9—H9	120.1
C2—C1—H1	119.8	O1—C10—C1	114.3 (3)
C2—C1—C10	120.4 (3)	C9—C10—O1	125.0 (3)
C10—C1—H1	119.8	C9—C10—C1	120.7 (3)
C1—C2—H2	119.5	O1—C11—H11A	109.8
C1—C2—C3	121.0 (3)	O1—C11—H11B	109.8
C3—C2—H2	119.5	O1—C11—C12	109.3 (3)
C4—C3—C2	123.2 (3)	H11A—C11—H11B	108.3
C8—C3—C2	118.1 (3)	C12—C11—H11A	109.8
C8—C3—C4	118.7 (3)	C12—C11—H11B	109.8
C3—C4—H4	119.5	O2—C12—O3	125.0 (4)
C5—C4—C3	121.0 (4)	O2—C12—C11	125.7 (3)
C5—C4—H4	119.5	O3—C12—C11	109.3 (3)
C4—C5—H5	119.6	O3—C13—H13A	110.2
C4—C5—C6	120.7 (4)	O3—C13—H13B	110.2
C6—C5—H5	119.6	O3—C13—C14	107.7 (3)
C5—C6—H6	120.0	H13A—C13—H13B	108.5
C7—C6—C5	120.0 (4)	C14—C13—H13A	110.2
C7—C6—H6	120.0	C14—C13—H13B	110.2
C6—C7—H7	119.6	C13—C14—H14A	109.5

C6—C7—C8	120.9 (4)	C13—C14—H14B	109.5
C8—C7—H7	119.6	C13—C14—H14C	109.5
C3—C8—C7	118.6 (3)	H14A—C14—H14B	109.5
C3—C8—C9	119.9 (3)	H14A—C14—H14C	109.5
C9—C8—C7	121.5 (3)	H14B—C14—H14C	109.5
C8—C9—H9	120.1		

O1—C11—C12—O2	2.2 (5)	C5—C6—C7—C8	−1.9 (6)
O1—C11—C12—O3	−175.8 (3)	C6—C7—C8—C3	1.8 (6)
C1—C2—C3—C4	−179.5 (4)	C6—C7—C8—C9	−180.0 (4)
C1—C2—C3—C8	−0.6 (6)	C7—C8—C9—C10	179.1 (3)
C2—C1—C10—O1	−179.9 (3)	C8—C3—C4—C5	1.4 (6)
C2—C1—C10—C9	−2.5 (6)	C8—C9—C10—O1	−179.6 (3)
C2—C3—C4—C5	−179.8 (4)	C8—C9—C10—C1	3.3 (6)
C2—C3—C8—C7	179.6 (3)	C10—O1—C11—C12	170.1 (3)
C2—C3—C8—C9	1.4 (6)	C10—C1—C2—C3	1.2 (6)
C3—C4—C5—C6	−1.5 (7)	C11—O1—C10—C1	−176.7 (3)
C3—C8—C9—C10	−2.7 (6)	C11—O1—C10—C9	6.1 (5)
C4—C3—C8—C7	−1.5 (6)	C12—O3—C13—C14	176.0 (3)
C4—C3—C8—C9	−179.7 (3)	C13—O3—C12—O2	2.2 (6)
C4—C5—C6—C7	1.8 (7)	C13—O3—C12—C11	−179.7 (3)