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n-Octanol

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Key indicators

Single-crystal X-ray study
T = 190 K
Mean σ(C–C) = 0.002 Å
R factor = 0.125
wR factor = 0.156
Data-to-parameter ratio = 22.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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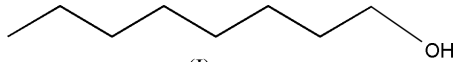
The structure of *n*-octanol, $C_8H_{17}OH$, at 150 K consists of infinite hydrogen-bonded chains forming a ribbon parallel to the *b* axis.

Comment

The low-molecular-weight aliphatic monoalcohols are liquid at room temperature. Methanol (CH_3OH; Allan *et al.*, 1998), ethanol (C_2H_5OH; Jönsson, 1976; Allan & Clark, 1999) and cyclobutanol ($C_4H_{10}OH$; McGregor *et al.*, 2003) form planar hydrogen-bonded ribbons in the solid state, while the bulkier tertiary butanol [$(CH_3)_3COH$; Steininger *et al.*, 1989] forms threefold helical hydrogen-bonded chains. At ambient pressure, phenol also forms threefold helical chains, while at 0.16 GPa and just above its normal melting point (313 K), it forms planar ribbons (Allan *et al.*, 2002). As part of a programme aimed at simplifying the growth of crystals from materials which are liquid at room temperature, we have looked at *n*-heptanol ($C_7H_{15}OH$) and *n*-octanol ($C_8H_{17}OH$). *n*-Heptanol could only be zone-crystallized, by a modification of the Bridgman technique (Bridgman, 1925), to an unindexable polycrystalline mass. *n*-Octanol, (I), was obtained as 'fair quality' single crystals accompanied by small satellite crystals. A previous examination of *n*-octanol crystals (Dunoyer & Ribaud, 1951) reported, on the basis of Debye–Scherrer photographs, a low-symmetry form just below the melting point, passing to an hexagonal form (a = 4.468 Å, c = 7.282 Å; ice I has a = 4.5 Å and c = 7.3 Å) between 248 and 215 K, after which the original low-symmetry cell reappeared.



(I)

In the present experiment, *n*-octanol was grown as a single crystal just below its melting point, and the temperature was then lowered to 150 K at a rate of 360 K per hour. There was no evidence of a phase transition.

In the low-temperature and ambient-pressure form of ethanol, the molecules form hydrogen-bonded ribbons, with the methyl group oriented somewhat towards the hydrogen-bonded backbone. This leads to a narrow ribbon with strained hydrogen-bonding angles. At ambient temperature and 3.0 GPa, the methyl groups of ethanol are coplanar with the backbone, lying fully extended on alternate sides. In *n*-octanol, the aliphatic chains are also coplanar, with the hydrogen-bonded backbone forming infinite wide ribbons parallel to the *b* axis. These ribbons pack side-by-side, with the terminal ethyl

groups parallel and in close contact, forming sheets of molecules.

Experimental

A single crystal of (I), which is a liquid at room temperature, was grown by keeping the compound under a cold nitrogen stream at just below its melting point, and slowly moving a small liquid zone up and down the sample. The temperature was then lowered for the main data collection.

Crystal data

$C_8H_{18}O$
M_r = 130.23
Monoclinic, $P2_1/n$
a = 4.2065 (2) Å
b = 5.1845 (2) Å
c = 38.9371 (18) Å
β = 91.723 (2)°
V = 848.78 (7) Å^3
Z = 4
D_x = 1.019 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1584 reflections
θ = 5–27°
μ = 0.06 mm^{-1}
T = 190 K
Cylinder, colourless
0.80 × 0.30 × 0.30 mm

Data collection

Nonius KappaCCD area-detector diffractometer
ω scans
Absorption correction: multi-scan, *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997)
T_{min} = 0.75, T_{max} = 0.98
11 803 measured reflections
1854 independent reflections
1011 reflections with $I \geq 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.4°
$h = -5 \rightarrow 5$
$k = -6 \rightarrow 5$
$l = -49 \rightarrow 50$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.125
$wR(F^2)$ = 0.157
S = 0.99
1854 reflections
82 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F) + 0.062 + 0.164P]$, where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.4352 (19)	C5—C6	1.526 (2)
C2—C3	1.511 (2)	C6—C7	1.524 (2)
C3—C4	1.530 (2)	C7—C8	1.526 (2)
C4—C5	1.524 (2)	C8—C9	1.518 (3)
O1—C2—C3	108.99 (14)	C5—C6—C7	114.18 (15)
C2—C3—C4	112.43 (14)	C6—C7—C8	113.72 (15)
C3—C4—C5	113.66 (14)	C7—C8—C9	113.58 (15)
C4—C5—C6	113.79 (14)		

The 'multi-scan' corrections applied by *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997) will also contain a contribution due to changes in the illuminated volume of the cylindrical sample. All H atoms were seen in a difference electron-density map. The hydroxyl H atom was placed as found, and the others were placed geometrically with U_{iso} values related to the adjacent atoms. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularise their geometry (C—H = 0.93–98 Å) and U_{iso}(H) values of 1.2–1.5 times U_{eq} of the adjacent atom, after which they were refined with riding constraints.

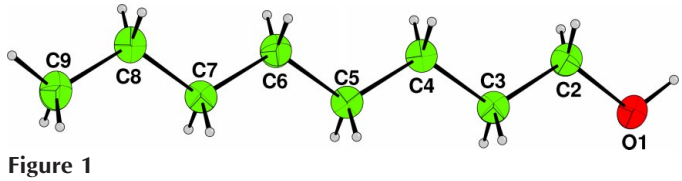


Figure 1
The title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are of arbitrary radii.

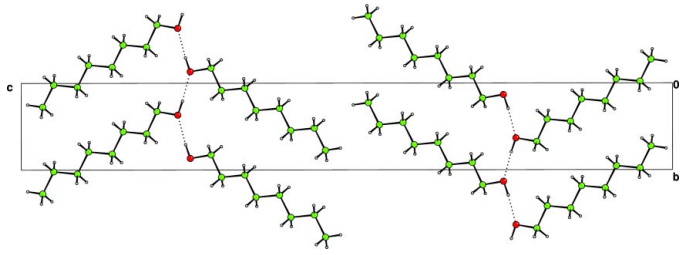


Figure 2
A packing diagram for (I), viewed along the *a* axis. The molecules are linked into ribbons by hydrogen bonds (dashed lines).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK*; data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

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supporting information

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$c = 38.9371$ (18) Å
$\beta = 91.723$ (2)°
$V = 848.78$ (7) Å^3
$Z = 4$
$F(000) = 296$
$D_x = 1.019$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1584 reflections
$\theta = 5$–27°
$\mu = 0.06$ mm^{-1}
$T = 190$ K
Cylinder, colourless
0.80 × 0.30 × 0.30 mm

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Nonius KappaCCD area-detector diffractometer
Graphite monochromator
ω scans
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11803 measured reflections
1854 independent reflections
1854 reflections with $I > -3u(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.4°$, $\theta_{min} = 5.1°$
$h = -5 \rightarrow 5$
$k = -6 \rightarrow 5$
$l = -49 \rightarrow 50$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.125$
$wR(F^2) = 0.157$
$S = 0.99$
1854 reflections
82 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F) + 0.062 + 0.164P]$, where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3510 (3)	0.3671 (2)	0.75958 (3)	0.0428
C2	0.5220 (4)	0.3257 (4)	0.79155 (4)	0.0359
C3	0.6035 (4)	0.5840 (3)	0.80749 (4)	0.0336
C4	0.7588 (4)	0.5578 (3)	0.84334 (4)	0.0345

C5	0.8392 (4)	0.8154 (3)	0.86032 (4)	0.0346
C6	0.9844 (4)	0.7901 (4)	0.89657 (4)	0.0352
C7	1.0667 (4)	1.0467 (3)	0.91372 (4)	0.0349
C8	1.2090 (4)	1.0191 (4)	0.95005 (4)	0.0399
C9	1.2932 (5)	1.2750 (4)	0.96696 (5)	0.0458
H21	0.3816	0.2307	0.8073	0.0432*
H22	0.7170	0.2261	0.7877	0.0429*
H31	0.4073	0.6837	0.8094	0.0404*
H32	0.7402	0.6816	0.7925	0.0398*
H41	0.6128	0.4650	0.8583	0.0408*
H42	0.9527	0.4482	0.8417	0.0413*
H51	0.6414	0.9186	0.8615	0.0409*
H52	0.9869	0.9134	0.8460	0.0397*
H61	0.8281	0.6997	0.9110	0.0422*
H62	1.1790	0.6822	0.8956	0.0419*
H71	0.8741	1.1527	0.9148	0.0420*
H72	1.2185	1.1390	0.8997	0.0420*
H81	1.0573	0.9292	0.9645	0.0489*
H82	1.4000	0.9104	0.9491	0.0489*
H91	1.3834	1.2490	0.9901	0.0542*
H92	1.1123	1.3909	0.9690	0.0550*
H93	1.4437	1.3628	0.9529	0.0557*
H1	0.2981	0.2074	0.7523	0.0686*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0530 (8)	0.0363 (8)	0.0381 (7)	−0.0003 (7)	−0.0160 (5)	−0.0012 (6)
C2	0.0387 (10)	0.0347 (12)	0.0339 (9)	0.0015 (9)	−0.0056 (7)	−0.0008 (8)
C3	0.0344 (9)	0.0328 (11)	0.0337 (9)	0.0006 (8)	−0.0017 (7)	0.0002 (8)
C4	0.0367 (10)	0.0325 (11)	0.0340 (9)	−0.0017 (8)	−0.0025 (7)	−0.0005 (8)
C5	0.0371 (10)	0.0324 (12)	0.0339 (9)	−0.0012 (8)	−0.0022 (8)	0.0009 (8)
C6	0.0371 (10)	0.0329 (11)	0.0352 (9)	0.0013 (8)	−0.0037 (8)	−0.0026 (8)
C7	0.0371 (10)	0.0312 (11)	0.0362 (9)	0.0000 (8)	−0.0027 (7)	−0.0006 (8)
C8	0.0435 (11)	0.0386 (12)	0.0372 (10)	−0.0030 (10)	−0.0048 (8)	−0.0025 (9)
C9	0.0524 (12)	0.0444 (13)	0.0400 (10)	−0.0013 (10)	−0.0083 (9)	−0.0069 (9)

Geometric parameters (Å, º)

O1—C2	1.4352 (19)	C5—H52	0.989
O1—H1	0.900	C6—C7	1.524 (2)
C2—C3	1.511 (2)	C6—H61	0.996
C2—H21	0.995	C6—H62	0.994
C2—H22	0.985	C7—C8	1.526 (2)
C3—C4	1.530 (2)	C7—H71	0.981
C3—H31	0.978	C7—H72	0.977
C3—H32	0.974	C8—C9	1.518 (3)
C4—C5	1.524 (2)	C8—H81	0.981

C4—H41	0.985	C8—H82	0.983
C4—H42	0.997	C9—H91	0.976
C5—C6	1.526 (2)	C9—H92	0.975
C5—H51	0.991	C9—H93	0.963

C2—O1—H1	104.271	C5—C6—C7	114.18 (15)
O1—C2—C3	108.99 (14)	C5—C6—H61	108.123
O1—C2—H21	108.491	C7—C6—H61	107.949
C3—C2—H21	108.500	C5—C6—H62	108.683
O1—C2—H22	110.091	C7—C6—H62	109.381
C3—C2—H22	110.370	H61—C6—H62	108.373
H21—C2—H22	110.347	C6—C7—C8	113.72 (15)
C2—C3—C4	112.43 (14)	C6—C7—H71	109.287
C2—C3—H31	108.570	C8—C7—H71	108.384
C4—C3—H31	108.326	C6—C7—H72	109.046
C2—C3—H32	110.178	C8—C7—H72	108.576
C4—C3—H32	110.478	H71—C7—H72	107.659
H31—C3—H32	106.656	C7—C8—C9	113.58 (15)
C3—C4—C5	113.66 (14)	C7—C8—H81	109.385
C3—C4—H41	109.118	C9—C8—H81	108.299
C5—C4—H41	107.744	C7—C8—H82	108.380
C3—C4—H42	108.716	C9—C8—H82	109.762
C5—C4—H42	110.818	H81—C8—H82	107.252
H41—C4—H42	106.525	C8—C9—H91	110.975
C4—C5—C6	113.79 (14)	C8—C9—H92	113.709
C4—C5—H51	108.527	H91—C9—H92	106.945
C6—C5—H51	108.452	C8—C9—H93	108.389
C4—C5—H52	109.870	H91—C9—H93	110.178
C6—C5—H52	109.031	H92—C9—H93	106.540
H51—C5—H52	106.934		