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Propane-1,3-diyl bis(4-aminobenzoate)

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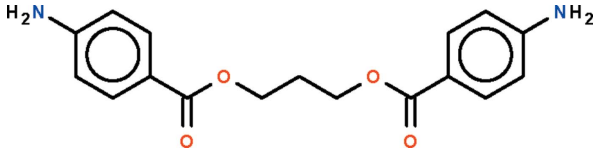
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.109; data-to-parameter ratio = 9.6.

Molecules of the title compound, $C_{17}H_{18}N_2O_4$, lie on a twofold rotation axis that passes through the central methylene C atom. The molecules adopt a 'V' shape and the trimethylene unit assumes a *gauche–gauche* conformation. The amino N atom shows a nonplanar coordination. Adjacent molecules are connected by N—H···O hydrogen bonds into chains running along [001]. Furthermore, N—H···N hydrogen bonds connect these chains into a three-dimensional network.

Related literature

For the crystal structure of 1,3-propandiyl-bis(benzoate), see: Pérez & Brisse (1977).



Experimental

Crystal data

$C_{17}H_{18}N_2O_4$
M_r = 314.33
Monoclinic, $C2$
a = 23.725 (5) Å
b = 4.5109 (9) Å
c = 8.2171 (17) Å
β = 107.173 (3)°
V = 840.2 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.35 × 0.35 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
3936 measured reflections
1082 independent reflections
788 reflections with $I > 2\sigma(I)$
R_{int} = 0.090

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.109
S = 0.96
1082 reflections
113 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···O2^{i}	0.86 (1)	2.15 (2)	2.958 (3)	157 (5)
N1—H12···N1^{ii}	0.86 (1)	2.25 (1)	3.104 (3)	169 (2)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; 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: BT5289).

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supplementary materials

Acta Cryst. (2010). E**66**, o1940 [**doi:10.1107/S1600536810026024**]

Propane-1,3-diyl bis(4-aminobenzoate)

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Comment

The chemical is a commercially available chemical that should be compable of condensing with carbonyl compounds to yield Schff bases; its special feature is its trimethylene portion, which assumes a *V* shape. The $C_{17}H_{18}N_2O_4$ molecule (Scheme I) lies on a twofold rotation axis that passes through the central methylene carbon atom; this symmetry element relates one 4-aminobenzoate unit to the other. The molecule assumes a *V* shape and the trimethylene portion assumes a *gauche–gauche* conformation. The amino nitrogen atom shows non-planar coordination (Fig. 1). Adjacent molecules are connected by N–H···O and N–H···N shydrogen bonds to form a three-dimensional network.

Experimental

The compound was returned unchanged but in a crystalline form in an unsuccessful condensation with *o*-vanillin in ethanol medium.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.95–0.99 Å, *U*(H) 1.2*U*(C)] and were included in the refinement in the riding model approximation. The amino H-atoms were located in a difference Fourier map, and were refined isotropically with a distance restraint of N–H 0.86±0.01 Å. 822 Friedel pairs were merged.

Figures

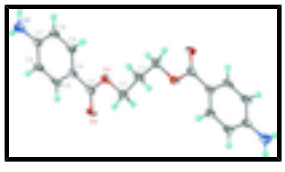

Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{17}H_{18}N_2O_4$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Propane-1,3-diyl bis(4-aminobenzoate)

Crystal data

$C_{17}H_{18}N_2O_4$	$F(000) = 332$
$M_r = 314.33$	$D_x = 1.242$ Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: C 2y	Cell parameters from 915 reflections
$a = 23.725$ (5) Å	θ = 2.6–26.8°
$b = 4.5109$ (9) Å	μ = 0.09 mm^{-1}
$c = 8.2171$ (17) Å	$T = 100$ K

β = 107.173 (3)°	Plate, yellow
V = 840.2 (3) Å^3	0.35 × 0.35 × 0.02 mm
Z = 2	

Data collection

Bruker SMART APEX diffractometer	788 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.090
graphite	θ_{max} = 27.5°, θ_{min} = 1.8°
ω scans	h = −30→29
3936 measured reflections	k = −5→5
1082 independent reflections	l = −10→10

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.043	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.109	H atoms treated by a mixture of independent and constrained refinement
S = 0.96	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
1082 reflections	$(\Delta/\sigma)_{max}$ = 0.001
113 parameters	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
3 restraints	$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.42724 (7)	0.4987 (4)	0.0488 (2)	0.0262 (5)	
O2	0.35969 (8)	0.7580 (5)	−0.1476 (2)	0.0304 (5)	
N1	0.29701 (11)	1.0783 (6)	0.5367 (3)	0.0298 (6)	
C1	0.5000	0.1862 (10)	0.0000	0.0279 (10)	
H1A	0.5095	0.0569	−0.0857	0.033*	0.50
H1B	0.4905	0.0569	0.0857	0.033*	0.50
C2	0.44676 (11)	0.3705 (7)	−0.0862 (3)	0.0263 (7)	
H2A	0.4572	0.5279	−0.1562	0.032*	
H2B	0.4153	0.2454	−0.1609	0.032*	
C3	0.38135 (11)	0.6876 (7)	0.0010 (3)	0.0244 (7)	
C4	0.36179 (11)	0.7924 (7)	0.1432 (3)	0.0228 (6)	
C5	0.31600 (11)	0.9969 (7)	0.1134 (3)	0.0260 (7)	
H5	0.2991	1.0721	0.0016	0.031*	
C6	0.29486 (12)	1.0917 (7)	0.2423 (3)	0.0286 (7)	
H6	0.2631	1.2289	0.2187	0.034*	
C7	0.31969 (11)	0.9879 (7)	0.4094 (3)	0.0252 (7)	

C8	0.36569 (11)	0.7851 (8)	0.4393 (3)	0.0295 (7)
H8	0.3830	0.7123	0.5514	0.035*
C9	0.38646 (11)	0.6885 (8)	0.3103 (3)	0.0282 (7)
H9	0.4179	0.5495	0.3338	0.034*
H11	0.3137 (17)	1.032 (12)	0.641 (2)	0.098 (16)*
H12	0.2748 (10)	1.233 (4)	0.519 (3)	0.025 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0204 (9)	0.0351 (12)	0.0206 (9)	0.0041 (10)	0.0021 (7)	0.0031 (9)
O2	0.0239 (10)	0.0453 (13)	0.0165 (9)	0.0042 (10)	−0.0024 (7)	0.0029 (10)
N1	0.0272 (14)	0.0364 (17)	0.0227 (13)	0.0056 (12)	0.0025 (11)	0.0016 (12)
C1	0.021 (2)	0.030 (3)	0.029 (2)	0.000	0.0034 (16)	0.000
C2	0.0205 (13)	0.0329 (17)	0.0243 (14)	−0.0040 (13)	0.0046 (11)	−0.0024 (13)
C3	0.0172 (13)	0.0302 (17)	0.0224 (13)	−0.0048 (13)	0.0005 (11)	0.0009 (13)
C4	0.0163 (12)	0.0304 (17)	0.0183 (12)	−0.0025 (12)	−0.0001 (10)	0.0023 (11)
C5	0.0190 (13)	0.0322 (17)	0.0193 (13)	−0.0007 (14)	−0.0058 (11)	0.0043 (13)
C6	0.0191 (14)	0.0368 (19)	0.0236 (14)	0.0029 (13)	−0.0031 (12)	0.0038 (13)
C7	0.0186 (13)	0.0335 (18)	0.0202 (13)	−0.0060 (14)	0.0006 (10)	0.0005 (13)
C8	0.0218 (14)	0.043 (2)	0.0179 (13)	0.0039 (14)	−0.0026 (11)	0.0090 (14)
C9	0.0181 (14)	0.0397 (19)	0.0237 (14)	0.0030 (14)	0.0012 (11)	0.0050 (14)

Geometric parameters (Å, °)

O1—C3	1.347 (3)	C3—C4	1.457 (4)
O1—C2	1.444 (3)	C4—C5	1.391 (4)
O2—C3	1.219 (3)	C4—C9	1.405 (3)
N1—C7	1.372 (3)	C5—C6	1.368 (4)
N1—H11	0.858 (10)	C5—H5	0.9500
N1—H12	0.861 (10)	C6—C7	1.405 (4)
C1—C2	1.503 (4)	C6—H6	0.9500
C1—C2^{i}	1.503 (4)	C7—C8	1.389 (4)
C1—H1A	0.9900	C8—C9	1.365 (4)
C1—H1B	0.9900	C8—H8	0.9500
C2—H2A	0.9900	C9—H9	0.9500
C2—H2B	0.9900		
C3—O1—C2	116.39 (19)	C5—C4—C9	118.1 (2)
C7—N1—H11	121 (3)	C5—C4—C3	119.4 (2)
C7—N1—H12	118.1 (19)	C9—C4—C3	122.4 (2)
H11—N1—H12	116 (4)	C6—C5—C4	121.1 (2)
C2—C1—C2^{i}	112.9 (4)	C6—C5—H5	119.4
C2—C1—H1A	109.0	C4—C5—H5	119.4
C2^{i}—C1—H1A	109.0	C5—C6—C7	120.6 (3)
C2—C1—H1B	109.0	C5—C6—H6	119.7
C2^{i}—C1—H1B	109.0	C7—C6—H6	119.7
H1A—C1—H1B	107.8	N1—C7—C8	121.7 (2)
O1—C2—C1	105.94 (18)	N1—C7—C6	120.0 (3)

O1—C2—H2A	110.5	C8—C7—C6	118.2 (2)
C1—C2—H2A	110.5	C9—C8—C7	121.2 (3)
O1—C2—H2B	110.5	C9—C8—H8	119.4
C1—C2—H2B	110.5	C7—C8—H8	119.4
H2A—C2—H2B	108.7	C8—C9—C4	120.7 (3)
O2—C3—O1	121.5 (2)	C8—C9—H9	119.7
O2—C3—C4	125.4 (3)	C4—C9—H9	119.7
O1—C3—C4	113.1 (2)		
C3—O1—C2—C1	176.5 (2)	C3—C4—C5—C6	177.4 (3)
C2^{i}—C1—C2—O1	−71.92 (18)	C4—C5—C6—C7	1.1 (4)
C2—O1—C3—O2	−3.8 (4)	C5—C6—C7—N1	−178.2 (3)
C2—O1—C3—C4	176.2 (2)	C5—C6—C7—C8	−0.6 (4)
O2—C3—C4—C5	−2.2 (4)	N1—C7—C8—C9	177.6 (3)
O1—C3—C4—C5	177.8 (3)	C6—C7—C8—C9	0.1 (5)
O2—C3—C4—C9	176.1 (3)	C7—C8—C9—C4	0.1 (5)
O1—C3—C4—C9	−4.0 (4)	C5—C4—C9—C8	0.3 (4)
C9—C4—C5—C6	−0.9 (4)	C3—C4—C9—C8	−177.9 (3)

Symmetry codes: (i) −*x*+1, *y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H11···O2^{ii}	0.86 (1)	2.15 (2)	2.958 (3)	157 (5)
N1—H12···N1^{iii}	0.86 (1)	2.25 (1)	3.104 (3)	169 (2)

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

Fig. 1