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N-{(*E*)-4-[(*E*)-(Dodecylimino)methyl]benzylidene}dodecan-1-imine

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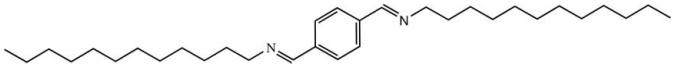
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.065; wR factor = 0.172; data-to-parameter ratio = 19.6.

The title compound, $C_{32}H_{56}N_2$, was synthesized by the reaction of terephthalaldehyde and dodecan-1-amine. The imines adopt *trans* conformations, with the two halves of the molecule related to each other by a centre of symmetry.

Related literature

For related literature, see: Sharaby (2007); Nishikawa *et al.* (1992). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{32}H_{56}N_2$
M_r = 468.80
Triclinic, $P\overline{1}$
a = 4.7370 (9) Å
b = 5.5190 (11) Å
c = 30.315 (6) Å
α = 91.18 (3)°
β = 93.44 (3)°
γ = 101.75 (3)°
V = 774.1 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.953, T_{max} = 0.964
3409 measured reflections
3020 independent reflections
1271 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.171
S = 1.06
3020 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
Selected bond lengths (Å).

N1—C13	1.252 (3)	N1—C12	1.454 (2)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank Professor Hua-Qin Wang, Analysis Centre, Nanjing University, for carrying out the X-ray crystallographic analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2115).

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N-{(*E*)-4-[(*E*)-(Dodecylimino)methyl]benzylidene}dodecan-1-imine

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S1. Comment

Schiff compounds and their derivatives containing long carbon chains are of great interest because of their surface active properties. They can be used as starting materials for producing polymers (Nishikawa, *et al.*, 1992). Certain imines coordinated to metals have also received a great deal of attention recently, due to their antibacterial and antifungal activities (Sharaby, 2007).

We report here the crystal structure of the title compound, (I). The molecular structure of (I) is shown in Fig. 1. The N—C double bonds and the benzene ring lie in the same plane. The double bonds conjugate with the benzene ring. The molecule is centrosymmetric. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

S2. Experimental

Terephthalaldehyde (5 mmol) and dodecan-1-amine (10 mmol) were dissolved in toluene (50 ml). The reaction mixture was allowed to reflux for 5 h, then left to cool to room temperature, filtered, and the solid was recrystallized from ethanol to give pure compound (I) (m.p. 333 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

S3. Refinement

All H atoms bonded to the C atoms were placed geometrically at distances of 0.93–0.97 Å and included in the refinement in riding motion approximation with U_{iso}(H) = 1.2 or 1.5U_{eq} of the carrier atom.

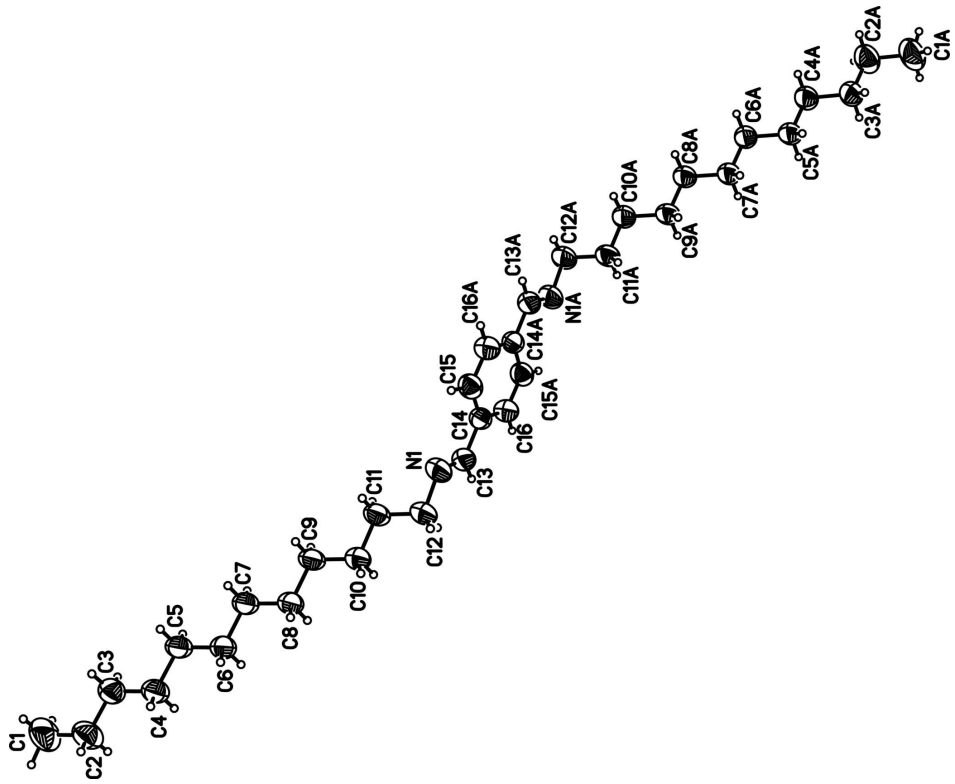

Figure 1

A view of the molecular structure of (I), showing the atom labelling scheme and ellipsoids at the 50% probability level.

_N_-{(_E_)-4-[(_E_)-(Dodecylimino)methyl]benzylidene}dodecan-\1-imine ?

Crystal data

$C_{32}H_{56}N_2$
M_r = 468.80
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 4.7370 (9) Å
b = 5.5190 (11) Å
c = 30.315 (6) Å
α = 91.18 (3)°
β = 93.44 (3)°
γ = 101.75 (3)°
V = 774.1 (3) Å^3
Z = 1
F(000) = 262
D_x = 1.006 Mg m^{-3}
Melting point = 332–333 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 9–13°
μ = 0.06 mm^{-1}
T = 298 K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.953, T_{max} = 0.964
3409 measured reflections
3020 independent reflections
1271 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 26.0°, θ_{min} = 1.4°
h = −5→5
k = −6→6
l = 0→37
3 standard reflections every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.171$
$S = 1.06$
3020 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.2538 (4)	−0.7333 (4)	0.10048 (7)	0.0778 (7)
C1	0.7923 (7)	1.2784 (5)	0.45915 (9)	0.1139 (11)
H1A	0.6948	1.3606	0.4799	0.171*
H1B	0.8934	1.3977	0.4400	0.171*
H1C	0.9278	1.1985	0.4749	0.171*
C2	0.5752 (6)	1.0886 (5)	0.43217 (9)	0.0957 (9)
H2A	0.4702	0.9734	0.4521	0.115*
H2B	0.4372	1.1718	0.4171	0.115*
C3	0.6950 (5)	0.9444 (4)	0.39859 (8)	0.0776 (7)
H3A	0.8330	0.8612	0.4136	0.093*
H3B	0.8002	1.0596	0.3786	0.093*
C4	0.4773 (5)	0.7540 (4)	0.37145 (8)	0.0748 (7)
H4A	0.3727	0.6382	0.3914	0.090*
H4B	0.3389	0.8370	0.3565	0.090*
C5	0.6000 (5)	0.6097 (4)	0.33745 (7)	0.0698 (7)
H5A	0.7367	0.5248	0.3524	0.084*
H5B	0.7060	0.7252	0.3176	0.084*
C6	0.3788 (5)	0.4215 (4)	0.31028 (7)	0.0683 (7)
H6A	0.2450	0.5068	0.2947	0.082*
H6B	0.2695	0.3084	0.3301	0.082*
C7	0.5035 (5)	0.2726 (4)	0.27696 (7)	0.0672 (7)
H7A	0.6154	0.3861	0.2574	0.081*
H7B	0.6351	0.1855	0.2926	0.081*
C8	0.2832 (5)	0.0869 (4)	0.24921 (7)	0.0665 (7)
H8A	0.1536	0.1742	0.2331	0.080*

H8B	0.1691	−0.0251	0.2687	0.080*
C9	0.4102 (5)	−0.0638 (4)	0.21653 (7)	0.0680 (7)
H9A	0.5357	−0.1544	0.2327	0.082*
H9B	0.5289	0.0487	0.1976	0.082*
C10	0.1910 (5)	−0.2461 (4)	0.18760 (7)	0.0706 (7)
H10A	0.0643	−0.3528	0.2064	0.085*
H10B	0.0734	−0.1553	0.1698	0.085*
C11	0.3247 (5)	−0.4049 (4)	0.15738 (7)	0.0679 (7)
H11A	0.4605	−0.2978	0.1400	0.081*
H11B	0.4328	−0.5029	0.1753	0.081*
C12	0.1100 (5)	−0.5762 (5)	0.12654 (8)	0.0814 (8)
H12A	−0.0327	−0.6788	0.1435	0.098*
H12B	0.0105	−0.4797	0.1069	0.098*
C13	0.2374 (5)	−0.7155 (4)	0.05935 (9)	0.0691 (7)
H13A	0.1336	−0.6041	0.0472	0.083*
C14	0.3736 (5)	−0.8616 (4)	0.02936 (8)	0.0599 (6)
C15	0.5322 (5)	−1.0284 (4)	0.04476 (8)	0.0662 (7)
H15A	0.5576	−1.0479	0.0750	0.079*
C16	0.3458 (5)	−0.8331 (4)	−0.01595 (9)	0.0705 (7)
H16A	0.2430	−0.7184	−0.0270	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0771 (14)	0.0880 (15)	0.0692 (14)	0.0179 (12)	0.0158 (12)	−0.0196 (12)
C1	0.129 (3)	0.098 (2)	0.105 (2)	0.007 (2)	0.003 (2)	−0.0417 (18)
C2	0.098 (2)	0.0910 (19)	0.092 (2)	0.0058 (17)	0.0204 (17)	−0.0272 (17)
C3	0.0739 (17)	0.0762 (16)	0.0810 (18)	0.0124 (14)	0.0088 (14)	−0.0160 (14)
C4	0.0687 (16)	0.0754 (16)	0.0798 (18)	0.0121 (14)	0.0158 (14)	−0.0155 (14)
C5	0.0625 (15)	0.0703 (15)	0.0782 (17)	0.0153 (13)	0.0171 (13)	−0.0122 (13)
C6	0.0582 (14)	0.0693 (15)	0.0765 (17)	0.0104 (13)	0.0124 (13)	−0.0116 (13)
C7	0.0611 (15)	0.0663 (14)	0.0754 (16)	0.0136 (13)	0.0157 (13)	−0.0104 (12)
C8	0.0625 (15)	0.0688 (14)	0.0696 (16)	0.0153 (13)	0.0137 (13)	−0.0091 (12)
C9	0.0643 (15)	0.0718 (15)	0.0713 (16)	0.0190 (13)	0.0196 (13)	−0.0097 (13)
C10	0.0614 (15)	0.0778 (16)	0.0726 (17)	0.0137 (14)	0.0135 (13)	−0.0134 (13)
C11	0.0690 (16)	0.0721 (15)	0.0657 (16)	0.0187 (13)	0.0189 (13)	−0.0079 (12)
C12	0.0737 (17)	0.0956 (18)	0.0769 (18)	0.0210 (16)	0.0184 (15)	−0.0256 (15)
C13	0.0552 (15)	0.0678 (15)	0.0824 (19)	0.0085 (13)	0.0094 (14)	−0.0150 (14)
C14	0.0494 (14)	0.0552 (14)	0.0723 (17)	0.0034 (12)	0.0120 (13)	−0.0098 (12)
C15	0.0690 (16)	0.0692 (15)	0.0596 (15)	0.0108 (14)	0.0099 (13)	−0.0034 (13)
C16	0.0670 (17)	0.0724 (16)	0.0747 (19)	0.0195 (14)	0.0098 (14)	−0.0049 (14)

Geometric parameters (Å, º)

N1—C13	1.252 (3)	C7—H7B	0.9700
N1—C12	1.454 (2)	C8—C9	1.509 (2)
C1—C2	1.500 (3)	C8—H8A	0.9700
C1—H1A	0.9600	C8—H8B	0.9700

C1—H1B	0.9600	C9—C10	1.513 (3)
C1—H1C	0.9600	C9—H9A	0.9700
C2—C3	1.487 (3)	C9—H9B	0.9700
C2—H2A	0.9700	C10—C11	1.507 (2)
C2—H2B	0.9700	C10—H10A	0.9700
C3—C4	1.505 (3)	C10—H10B	0.9700
C3—H3A	0.9700	C11—C12	1.503 (3)
C3—H3B	0.9700	C11—H11A	0.9700
C4—C5	1.504 (2)	C11—H11B	0.9700
C4—H4A	0.9700	C12—H12A	0.9700
C4—H4B	0.9700	C12—H12B	0.9700
C5—C6	1.508 (3)	C13—C14	1.464 (3)
C5—H5A	0.9700	C13—H13A	0.9300
C5—H5B	0.9700	C14—C15	1.374 (3)
C6—C7	1.510 (2)	C14—C16	1.387 (3)
C6—H6A	0.9700	C15—C16^{i}	1.376 (3)
C6—H6B	0.9700	C15—H15A	0.9300
C7—C8	1.507 (3)	C16—C15^{i}	1.376 (3)
C7—H7A	0.9700	C16—H16A	0.9300

C13—N1—C12	117.7 (2)	C7—C8—C9	114.44 (18)
C2—C1—H1A	109.5	C7—C8—H8A	108.7
C2—C1—H1B	109.5	C9—C8—H8A	108.7
H1A—C1—H1B	109.5	C7—C8—H8B	108.7
C2—C1—H1C	109.5	C9—C8—H8B	108.7
H1A—C1—H1C	109.5	H8A—C8—H8B	107.6
H1B—C1—H1C	109.5	C8—C9—C10	114.96 (18)
C3—C2—C1	115.7 (2)	C8—C9—H9A	108.5
C3—C2—H2A	108.4	C10—C9—H9A	108.5
C1—C2—H2A	108.4	C8—C9—H9B	108.5
C3—C2—H2B	108.4	C10—C9—H9B	108.5
C1—C2—H2B	108.4	H9A—C9—H9B	107.5
H2A—C2—H2B	107.4	C11—C10—C9	113.62 (18)
C2—C3—C4	115.7 (2)	C11—C10—H10A	108.8
C2—C3—H3A	108.3	C9—C10—H10A	108.8
C4—C3—H3A	108.3	C11—C10—H10B	108.8
C2—C3—H3B	108.3	C9—C10—H10B	108.8
C4—C3—H3B	108.3	H10A—C10—H10B	107.7
H3A—C3—H3B	107.4	C12—C11—C10	114.14 (18)
C5—C4—C3	115.43 (18)	C12—C11—H11A	108.7
C5—C4—H4A	108.4	C10—C11—H11A	108.7
C3—C4—H4A	108.4	C12—C11—H11B	108.7
C5—C4—H4B	108.4	C10—C11—H11B	108.7
C3—C4—H4B	108.4	H11A—C11—H11B	107.6
H4A—C4—H4B	107.5	N1—C12—C11	110.77 (19)
C4—C5—C6	114.74 (17)	N1—C12—H12A	109.5
C4—C5—H5A	108.6	C11—C12—H12A	109.5
C6—C5—H5A	108.6	N1—C12—H12B	109.5

C4—C5—H5B	108.6	C11—C12—H12B	109.5
C6—C5—H5B	108.6	H12A—C12—H12B	108.1
H5A—C5—H5B	107.6	N1—C13—C14	123.2 (3)
C5—C6—C7	114.56 (17)	N1—C13—H13A	118.4
C5—C6—H6A	108.6	C14—C13—H13A	118.4
C7—C6—H6A	108.6	C15—C14—C16	118.0 (2)
C5—C6—H6B	108.6	C15—C14—C13	121.8 (2)
C7—C6—H6B	108.6	C16—C14—C13	120.2 (2)
H6A—C6—H6B	107.6	C14—C15—C16^{i}	120.9 (2)
C8—C7—C6	114.84 (18)	C14—C15—H15A	119.6
C8—C7—H7A	108.6	C16^{i}—C15—H15A	119.6
C6—C7—H7A	108.6	C15^{i}—C16—C14	121.1 (2)
C8—C7—H7B	108.6	C15^{i}—C16—H16A	119.5
C6—C7—H7B	108.6	C14—C16—H16A	119.5
H7A—C7—H7B	107.5		

C1—C2—C3—C4	−179.9 (2)	C13—N1—C12—C11	−118.5 (3)
C2—C3—C4—C5	179.8 (2)	C10—C11—C12—N1	−176.5 (2)
C3—C4—C5—C6	−179.4 (2)	C12—N1—C13—C14	179.61 (18)
C4—C5—C6—C7	−178.6 (2)	N1—C13—C14—C15	−0.5 (3)
C5—C6—C7—C8	−179.1 (2)	N1—C13—C14—C16	179.8 (2)
C6—C7—C8—C9	−179.04 (19)	C16—C14—C15—C16^{i}	−1.5 (3)
C7—C8—C9—C10	−178.4 (2)	C13—C14—C15—C16^{i}	178.85 (19)
C8—C9—C10—C11	−176.34 (19)	C15—C14—C16—C15^{i}	1.5 (3)
C9—C10—C11—C12	−176.5 (2)	C13—C14—C16—C15^{i}	−178.85 (19)

Symmetry code: (i) $-x+1, -y-2, -z$.