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(1*E*)-1-[4-(Dimethylamino)phenyl]pent-1-en-3-one

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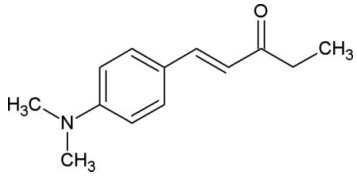
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.234; data-to-parameter ratio = 20.0.

The title molecule, $C_{13}H_{17}NO$, is close to planar: the dihedral angle betweent the dimethyl amino group and the benzene ring is 7.94 (19)°. No significant intermolecular interactions are observed in the crystal structure.

Related literature

For background to the pharmacological effects of chalcones, see: Nielsen *et al.* (1998) and for their use as synthetic intermediates, see: Mukhtari *et al.* (1999). For related structures, see: Nesterov *et al.* (2007); Arshad *et al.* (2008).



Experimental

Crystal data

$C_{13}H_{17}NO$
M_r = 203.28
Monoclinic, $P2_1/c$
a = 12.6079 (14) Å
b = 15.1331 (17) Å
c = 6.2182 (6) Å
β = 100.036 (5)°
V = 1168.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 K
0.37 × 0.33 × 0.19 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.974, T_{max} = 0.986
12449 measured reflections
2779 independent reflections
1051 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.234
S = 0.93
2779 reflections
139 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5213).

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supporting information

Acta Cryst. (2009). E**65**, o3063 [doi:10.1107/S1600536809046972]

(1*E*)-1-[4-(Dimethylamino)phenyl]pent-1-en-3-one

Muhammad Nadeem Asghar, Islam Ullah Khan, Muhammad Nadeem Arshad and Jeveria Rehman

S1. Comment

Chalcones are biologically active compounds (e.g. Nielsen *et al.*, 1998) and have also been used as intermediates for the synthesis of 4-thiazolidinones (Mukhtari *et al.*, 1999).

The title compound (I) was synthesized by the condensation reaction of 4-(dimethylamino)benzaldehyde and 2-butanol. The molecule is structurally related to the 3,5-Bis[4-(dimethylamino)benzylidene]-1-propyl-4-piperidone(II) (Nesterov *et al.*, 2007) and (1E,4E)-1,5-Bis(4-methylphenyl)penta-1,4-dien-3-one(III) (Arshad *et al.*, 2008). The compound is almost planer while the dimethyl amino moity is oriented at dihedral angle of 7.94 (0.19) ° to the benzene ring. No significant hydrogen bonding interaction is found in the crystal structure.

S2. Experimental

Sodium hydroxide (0.8 g, 0.0208 mmol) was dissolved in distilled water (10 ml) and ethanol (8 ml) in a round bottom flask. The solution was cooled to room temperature. Half of the mixture of 4-(dimethylamino)benzaldehyde (1 g, 0.0083 mmol) and 2-butanol (0.60 g, 0.0083 mmol) were added to the above solution and stirred at room temperature for 15 minute then the remaining mixture was added and stirred for 2 h under the same conditions. Yellow precipitate obtained was filtered and washed with cold water. The washed precipitate was crystallized in acetone under slow evaporation to yield yellow rods of (I).

S3. Refinement

The H-atoms for aromatic (C—H = 0.93), methyl (C—H = 0.96) and methylene (C—H = 0.97) carbon atoms were refined geometrically and treated as riding atoms: with U_{iso}(H) = 1.2U_{eq} for aromatic and methylene carbons and U_{iso}(H) = 1.5U_{eq} for methyl carbon atoms.

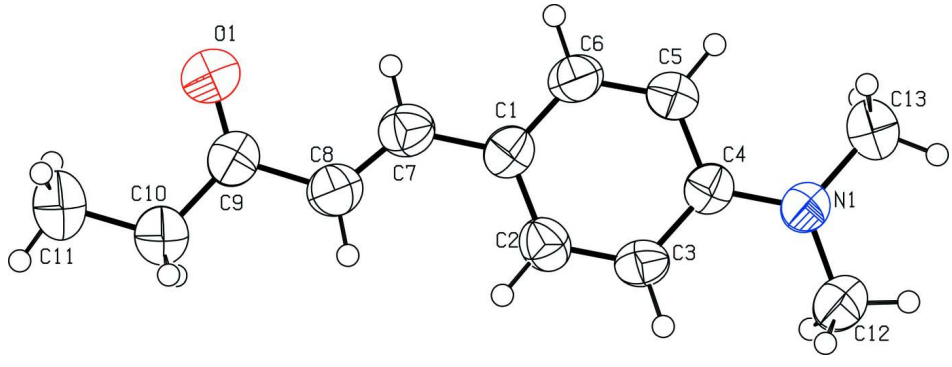

Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at 50% probability level.

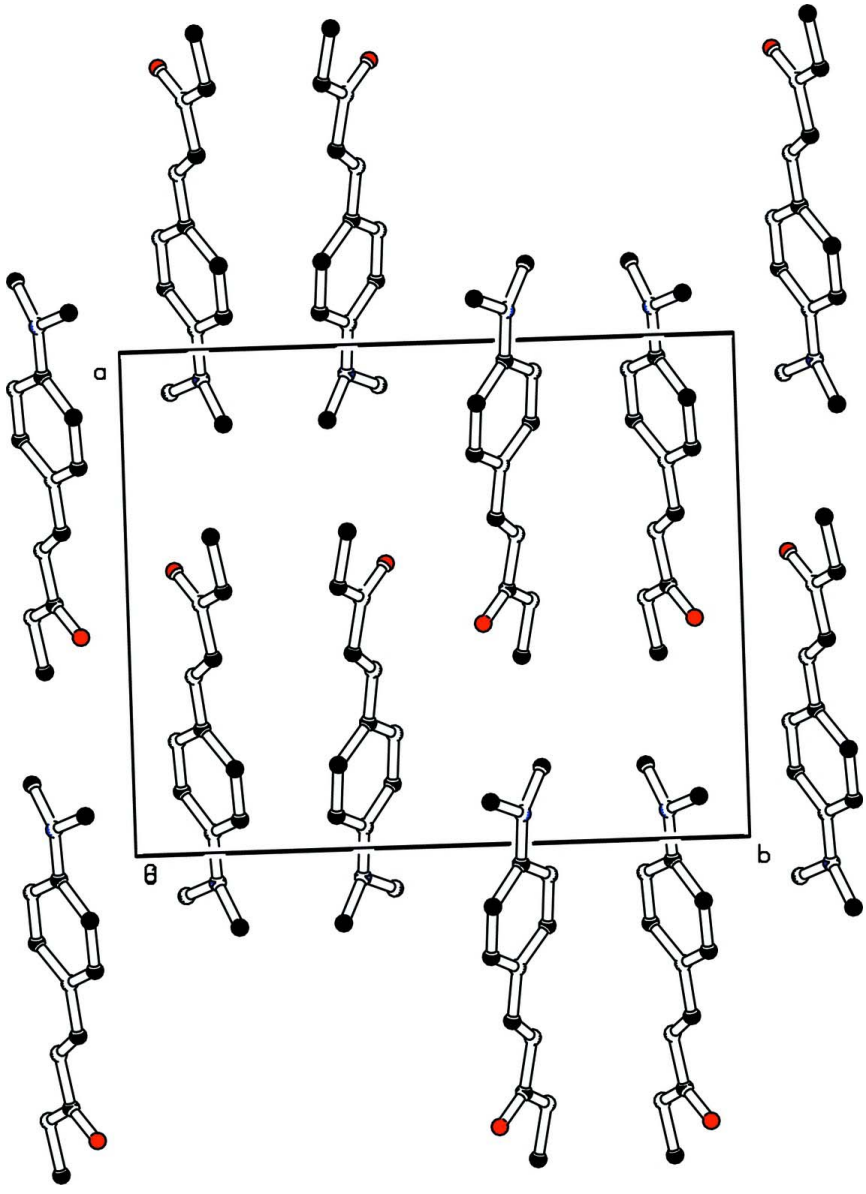

Figure 2

Unit cell packing diagram.

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$c = 6.2182\ (6)$ Å
$\beta = 100.036\ (5)°$
$V = 1168.3\ (2)$ Å^3
$Z = 4$
$F(000) = 440$
$D_x = 1.156$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1287 reflections

θ = 2.7–21.9°
μ = 0.07 mm^{-1}
T = 296 K

Rod, yellow
0.37 × 0.33 × 0.19 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.974, T_{max} = 0.986

12449 measured reflections
2779 independent reflections
1051 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.9°, θ_{min} = 1.6°
h = −16→16
k = −19→19
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.234
S = 0.93
2779 reflections
139 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
$w = 1/[\sigma^2(F_o^2) + (0.1169P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	−0.05777 (18)	0.36843 (15)	1.1136 (4)	0.0547 (7)
O1	0.5620 (2)	0.42215 (19)	0.7701 (4)	0.1083 (10)
C1	0.2477 (2)	0.38513 (17)	0.9326 (4)	0.0519 (7)
C2	0.1656 (2)	0.33421 (18)	0.8155 (5)	0.0563 (8)
H2	0.1790	0.3029	0.6944	0.068*
C3	0.0653 (2)	0.32866 (18)	0.8728 (4)	0.0529 (8)
H3	0.0121	0.2947	0.7888	0.063*
C4	0.0421 (2)	0.37361 (17)	1.0567 (4)	0.0472 (7)
C5	0.1260 (2)	0.42154 (18)	1.1781 (4)	0.0539 (8)
H5	0.1145	0.4506	1.3037	0.065*
C6	0.2252 (2)	0.42703 (19)	1.1174 (5)	0.0577 (8)
H6	0.2790	0.4599	1.2029	0.069*
C7	0.3527 (2)	0.39618 (19)	0.8680 (5)	0.0601 (8)

H7	0.4020	0.4306	0.9604	0.072*
C8	0.3862 (2)	0.3640 (2)	0.6976 (5)	0.0628 (8)
H8	0.3395	0.3287	0.6017	0.075*
C9	0.4952 (3)	0.3811 (2)	0.6492 (5)	0.0633 (9)
C10	0.5181 (3)	0.3440 (3)	0.4438 (5)	0.0832 (11)
H10A	0.4650	0.3670	0.3252	0.100*
H10B	0.5081	0.2805	0.4476	0.100*
C11	0.6267 (3)	0.3614 (3)	0.3914 (6)	0.0963 (12)
H11A	0.6404	0.4238	0.3967	0.144*
H11B	0.6299	0.3396	0.2477	0.144*
H11C	0.6801	0.3319	0.4960	0.144*
C12	−0.1486 (2)	0.3348 (2)	0.9610 (5)	0.0707 (9)
H12A	−0.1530	0.3648	0.8236	0.106*
H12B	−0.2137	0.3447	1.0178	0.106*
H12C	−0.1395	0.2726	0.9402	0.106*
C13	−0.0816 (3)	0.4196 (2)	1.2966 (5)	0.0650 (9)
H13A	−0.0345	0.4018	1.4277	0.097*
H13B	−0.1550	0.4097	1.3127	0.097*
H13C	−0.0711	0.4813	1.2706	0.097*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0483 (15)	0.0563 (15)	0.0600 (14)	−0.0042 (11)	0.0104 (11)	−0.0056 (12)
O1	0.0766 (18)	0.148 (3)	0.1051 (19)	−0.0394 (16)	0.0280 (15)	−0.0576 (18)
C1	0.0488 (17)	0.0481 (17)	0.0581 (17)	−0.0005 (13)	0.0077 (14)	0.0043 (14)
C2	0.063 (2)	0.0501 (18)	0.0582 (17)	0.0022 (15)	0.0170 (15)	−0.0019 (14)
C3	0.0561 (19)	0.0445 (17)	0.0564 (17)	−0.0048 (13)	0.0049 (14)	−0.0052 (13)
C4	0.0492 (17)	0.0371 (15)	0.0555 (16)	−0.0001 (13)	0.0094 (14)	0.0048 (13)
C5	0.057 (2)	0.0529 (18)	0.0518 (16)	−0.0017 (14)	0.0089 (14)	−0.0070 (13)
C6	0.0516 (19)	0.0588 (19)	0.0598 (18)	−0.0061 (14)	0.0015 (14)	−0.0066 (15)
C7	0.058 (2)	0.058 (2)	0.0621 (18)	0.0016 (15)	0.0047 (15)	−0.0015 (15)
C8	0.058 (2)	0.064 (2)	0.0653 (19)	−0.0031 (16)	0.0067 (16)	−0.0058 (16)
C9	0.054 (2)	0.068 (2)	0.0689 (19)	−0.0046 (16)	0.0129 (16)	−0.0040 (16)
C10	0.064 (2)	0.111 (3)	0.077 (2)	−0.007 (2)	0.0190 (17)	−0.019 (2)
C11	0.072 (2)	0.125 (3)	0.099 (3)	0.000 (2)	0.034 (2)	−0.017 (2)
C12	0.056 (2)	0.075 (2)	0.082 (2)	−0.0110 (17)	0.0134 (17)	−0.0093 (18)
C13	0.067 (2)	0.066 (2)	0.0651 (19)	0.0049 (16)	0.0215 (15)	0.0024 (16)

Geometric parameters (Å, º)

N1—C4	1.368 (3)	C7—H7	0.9300
N1—C12	1.447 (3)	C8—C9	1.480 (4)
N1—C13	1.451 (4)	C8—H8	0.9300
O1—C9	1.200 (3)	C9—C10	1.469 (4)
C1—C6	1.385 (4)	C10—C11	1.485 (4)
C1—C2	1.390 (4)	C10—H10A	0.9700
C1—C7	1.458 (4)	C10—H10B	0.9700

C2—C3	1.375 (4)	C11—H11A	0.9600
C2—H2	0.9300	C11—H11B	0.9600
C3—C4	1.404 (3)	C11—H11C	0.9600
C3—H3	0.9300	C12—H12A	0.9600
C4—C5	1.391 (4)	C12—H12B	0.9600
C5—C6	1.370 (4)	C12—H12C	0.9600
C5—H5	0.9300	C13—H13A	0.9600
C6—H6	0.9300	C13—H13B	0.9600
C7—C8	1.302 (4)	C13—H13C	0.9600

C4—N1—C12	120.6 (2)	O1—C9—C10	121.3 (3)
C4—N1—C13	119.9 (2)	O1—C9—C8	122.6 (3)
C12—N1—C13	117.0 (2)	C10—C9—C8	116.1 (3)
C6—C1—C2	116.5 (3)	C9—C10—C11	116.9 (3)
C6—C1—C7	120.2 (3)	C9—C10—H10A	108.1
C2—C1—C7	123.2 (3)	C11—C10—H10A	108.1
C3—C2—C1	122.2 (3)	C9—C10—H10B	108.1
C3—C2—H2	118.9	C11—C10—H10B	108.1
C1—C2—H2	118.9	H10A—C10—H10B	107.3
C2—C3—C4	120.8 (3)	C10—C11—H11A	109.5
C2—C3—H3	119.6	C10—C11—H11B	109.5
C4—C3—H3	119.6	H11A—C11—H11B	109.5
N1—C4—C5	122.4 (2)	C10—C11—H11C	109.5
N1—C4—C3	120.9 (3)	H11A—C11—H11C	109.5
C5—C4—C3	116.6 (3)	H11B—C11—H11C	109.5
C6—C5—C4	121.7 (3)	N1—C12—H12A	109.5
C6—C5—H5	119.1	N1—C12—H12B	109.5
C4—C5—H5	119.1	H12A—C12—H12B	109.5
C5—C6—C1	122.0 (3)	N1—C12—H12C	109.5
C5—C6—H6	119.0	H12A—C12—H12C	109.5
C1—C6—H6	119.0	H12B—C12—H12C	109.5
C8—C7—C1	128.4 (3)	N1—C13—H13A	109.5
C8—C7—H7	115.8	N1—C13—H13B	109.5
C1—C7—H7	115.8	H13A—C13—H13B	109.5
C7—C8—C9	123.0 (3)	N1—C13—H13C	109.5
C7—C8—H8	118.5	H13A—C13—H13C	109.5
C9—C8—H8	118.5	H13B—C13—H13C	109.5

C6—C1—C2—C3	3.0 (4)	C4—C5—C6—C1	−0.2 (4)
C7—C1—C2—C3	−176.3 (3)	C2—C1—C6—C5	−2.4 (4)
C1—C2—C3—C4	−1.1 (4)	C7—C1—C6—C5	177.0 (3)
C12—N1—C4—C5	166.5 (3)	C6—C1—C7—C8	−177.9 (3)
C13—N1—C4—C5	4.9 (4)	C2—C1—C7—C8	1.4 (5)
C12—N1—C4—C3	−14.8 (4)	C1—C7—C8—C9	179.4 (3)
C13—N1—C4—C3	−176.4 (2)	C7—C8—C9—O1	3.8 (5)
C2—C3—C4—N1	179.8 (3)	C7—C8—C9—C10	−176.6 (3)
C2—C3—C4—C5	−1.4 (4)	O1—C9—C10—C11	−1.2 (5)
N1—C4—C5—C6	−179.1 (2)	C8—C9—C10—C11	179.3 (3)

C3—C4—C5—C6	2.1 (4)