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ISSN 2414-3146

2-(5-Methyl-1-benzofuran-3-yl)-*N*-(2-phenylethyl)-acetamide

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Received 31 January 2017
Accepted 7 February 2017

Edited by J. Simpson, University of Otago, New Zealand

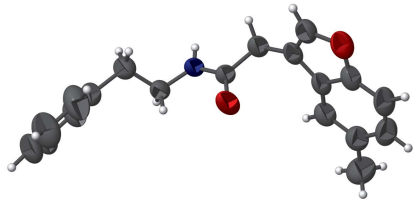
Keywords: crystal structure; benzofuran; hydrogen bonding; π–π stacking.

CCDC reference: 1503758

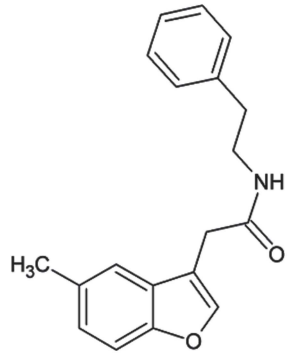
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{19}H_{19}NO_2$, is non-planar with the phenyl ring of the phenethylacetamide residue inclined to the benzofuran ring system by 84.8 (3)°. The methyl group lies in the plane of the fused ring system [C—C—C—C torsion angle = −179.6 (3)°]. In the crystal, N—H···O hydrogen bonds link the molecules into chains along the *a*-axis direction. π–π stacking interactions with a centroid-to-centroid distances of 3.497 (3) Å further stabilize the structure, stacking the molecules along *a*.

3D view



Chemical scheme



Structure description

Benzofuran derivatives with an amide linkage have attracted attention due to their wide range of biological activities. These include acting as melatonin receptor selective ligands (Wallez *et al.*, 2002), glycogen synthase kinase 3β inhibitors, which suppress proliferation and survival of pancreatic cancer cells (Gaisina *et al.*, 2009), and ischemic cell death inhibitors (Suh *et al.*, 2010). They are also used as antitubercular and antifungal (Telvekar *et al.*, 2012) or anticonvulsant agents (Shakya *et al.*, 2016). They inhibit monoamine oxidase (Pisani *et al.*, 2013), the hepatitis C virus (Bowman *et al.*, 2015) and NF-kB activity (Choi *et al.*, 2016). Other pharmaceutical applications include the treatment of cognitive disorders (Mazurov *et al.*, 2012) and as anti-oestrogen breast cancer agents (Li *et al.*, 2013). Chemically they are used as intermediates for the synthesis of morphine alkaloids (France *et al.*, 2008).

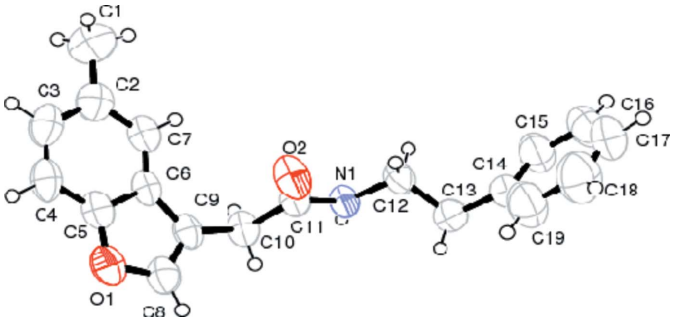


Figure 1
The molecular structure of the title compound, showing 40% probability displacement ellipsoids and the atom numbering.

The title compound (Fig. 1) is non-planar. The C14–C18 phenyl ring of the phenethylacetamide residue is inclined to the planar benzofuran ring system by 84.8 (3)°. The r.m.s. deviation from the plane through the ten atoms of the benzofuran ring system is 0.011 Å. The molecular structure is similar to that observed for 2-(5-methyl-1-benzofuran-3-yl)-acetic acid (Ramprasad *et al.*, 2016).

In the crystal, N1—H1···O2 hydrogen bonds (Table 1) link the molecules into chains along the *a*-axis direction. A π–π stacking interaction [$Cg\cdots Cg^{ii}$ = 3.497 (3) Å, *Cg* is the centroid of the O1/C5/C6/C8/C9 ring; symmetry code: (ii) $2-x, -y, 2-z$] further stabilizes the structure, Fig. 2, stacking the molecules along *a*.

Synthesis and crystallization

5-Methyl-benzofuran-3-acetic acid (10 mmol) (Basanagouda *et al.*, 2015; Uriarte *et al.*, 1995) was refluxed with phenyl-ethylamine (10 mmol) in benzene (30 ml) for 7 h (monitored by TLC). The solvent was removed to obtain a colourless solid, which was crystallized from a mixture of benzene and petroleum ether (1:1). Crystals suitable for diffraction studies were obtained by the slow evaporation of a solvent mixture of benzene and petroleum ether (1:1).

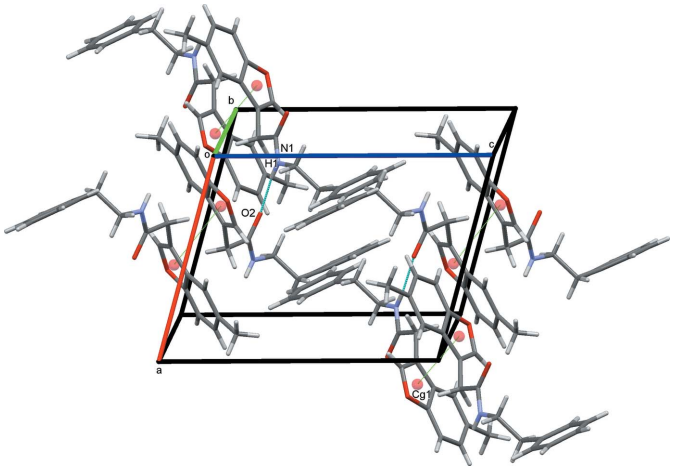


Figure 2
Packing diagram viewed along the *b* axis, with hydrogen bonds drawn as dashed lines. Ring centroids are shown as coloured spheres and π–π contacts as dotted lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.79 (3)	2.06 (3)	2.849 (3)	173 (3)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{19}NO_2$
M_r	293.35
Crystal system, space group	Monoclinic, $P2_1/a$
Temperature (K)	293
a, *b*, *c* (Å)	9.440 (6), 14.6051 (15), 12.321 (2)
β (°)	105.68 (3)
V (Å^3)	1635.5 (10)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.61
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Enraf–Nonius CAD-4
Absorption correction	ψ scan (*CAD-4 Software*; Enraf–Nonius, 1989)
T_{min}, T_{max}	0.884, 0.983
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2962, 2777, 1611
R_{int}	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.588
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.063, 0.169, 1.04
No. of reflections	2777
No. of parameters	205
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.20

Computer programs: *CAD-4 Software* (Enraf–Nonius, 1989), *XCAD4* (Harms & Wocadlo, 1995), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank the SAIF IIT Madras, Chennai, India, for the data collection.

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full crystallographic data

IUCrData (2017). **2**, x170200 [https://doi.org/10.1107/S2414314617002000]

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Crystal data

$C_{19}H_{19}NO_2$
M_r = 293.35
Monoclinic, $P2_1/a$
Hall symbol: -P 2yab
a = 9.440 (6) Å
b = 14.6051 (15) Å
c = 12.321 (2) Å
β = 105.68 (3)°
V = 1635.5 (10) Å^3
Z = 4
$F(000)$ = 624
D_x = 1.191 Mg m^{-3}
Melting point: 374 K
Cu $K\alpha$ radiation, λ = 1.54180 Å
Cell parameters from 25 reflections
θ = 20–30°
μ = 0.61 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–2τ scan
Absorption correction: ψ scan (CAD-4 Software; Enraf–Nonius, 1989)
T_{min} = 0.884, T_{max} = 0.983
2962 measured reflections
2777 independent reflections
1611 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 65.0°, θ_{min} = 3.7°
h = 0→11
k = 0→17
l = −14→13
2 standard reflections every 3600 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.169
S = 1.04
2777 reflections
205 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 0.197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0138 (11)

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	1.4210 (5)	0.2541 (3)	1.2438 (3)	0.1106 (13)
H1A	1.4362	0.2308	1.3189	0.166*
H1B	1.3544	0.3051	1.2328	0.166*
H1C	1.5134	0.2737	1.2331	0.166*
C2	1.3564 (4)	0.1798 (2)	1.1596 (3)	0.0759 (9)
C3	1.4336 (4)	0.0988 (3)	1.1569 (3)	0.0846 (11)
H3	1.5253	0.0914	1.2082	0.101*
C4	1.3806 (4)	0.0296 (3)	1.0820 (3)	0.0785 (10)
H4	1.4336	−0.0241	1.0817	0.094*
C5	1.2452 (3)	0.0433 (2)	1.0074 (3)	0.0628 (8)
C6	1.1619 (3)	0.12179 (19)	1.0061 (2)	0.0563 (8)
C7	1.2192 (3)	0.1905 (2)	1.0831 (3)	0.0671 (8)
H7	1.1656	0.2438	1.0836	0.081*
C8	1.0405 (3)	0.0264 (2)	0.8746 (3)	0.0699 (9)
H8	0.9679	0.0007	0.8160	0.084*
C9	1.0287 (3)	0.10883 (19)	0.9184 (2)	0.0582 (8)
C10	0.8999 (3)	0.1722 (2)	0.8871 (3)	0.0641 (8)
H10A	0.8761	0.1916	0.9553	0.077*
H10B	0.8159	0.1388	0.8416	0.077*
C11	0.9241 (3)	0.25580 (18)	0.8229 (2)	0.0516 (7)
C12	0.8114 (3)	0.39129 (18)	0.7207 (3)	0.0611 (8)
H12A	0.9075	0.3964	0.7069	0.073*
H12B	0.7981	0.4444	0.7643	0.073*
C13	0.6974 (4)	0.3930 (2)	0.6110 (3)	0.0842 (10)
H13A	0.6012	0.3994	0.6241	0.101*
H13B	0.6992	0.3354	0.5721	0.101*
C14	0.7222 (4)	0.4706 (2)	0.5379 (3)	0.0712 (9)
C15	0.6933 (5)	0.5581 (3)	0.5605 (3)	0.0926 (11)
H15	0.6502	0.5700	0.6186	0.111*
C16	0.7264 (5)	0.6302 (3)	0.4992 (4)	0.1059 (13)
H16	0.7048	0.6898	0.5163	0.127*
C17	0.7900 (5)	0.6152 (3)	0.4146 (4)	0.1068 (14)
H17	0.8148	0.6640	0.3747	0.128*
C18	0.8165 (6)	0.5295 (4)	0.3895 (4)	0.1203 (15)
H18	0.8575	0.5184	0.3300	0.144*

C19	0.7842 (5)	0.4564 (3)	0.4501 (4)	0.1108 (14)
H19	0.8047	0.3971	0.4315	0.133*
N1	0.8092 (2)	0.31022 (16)	0.7869 (2)	0.0546 (7)
O1	1.1717 (2)	−0.01657 (14)	0.92533 (19)	0.0737 (6)
O2	1.04377 (19)	0.27316 (14)	0.8051 (2)	0.0804 (7)
H1	0.736 (4)	0.290 (2)	0.797 (3)	0.077 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.105 (3)	0.123 (3)	0.099 (3)	−0.008 (3)	0.019 (2)	−0.014 (3)
C2	0.072 (2)	0.085 (2)	0.075 (2)	0.0026 (19)	0.0275 (18)	0.0129 (19)
C3	0.063 (2)	0.104 (3)	0.085 (3)	0.018 (2)	0.0183 (19)	0.024 (2)
C4	0.068 (2)	0.084 (2)	0.089 (2)	0.0300 (19)	0.0306 (19)	0.025 (2)
C5	0.0632 (19)	0.0623 (18)	0.071 (2)	0.0153 (15)	0.0329 (16)	0.0176 (16)
C6	0.0538 (17)	0.0561 (17)	0.0680 (19)	0.0106 (14)	0.0321 (15)	0.0174 (15)
C7	0.0630 (19)	0.0658 (19)	0.081 (2)	0.0104 (16)	0.0336 (17)	0.0132 (18)
C8	0.066 (2)	0.067 (2)	0.079 (2)	0.0054 (16)	0.0227 (17)	0.0184 (17)
C9	0.0550 (17)	0.0561 (18)	0.071 (2)	0.0068 (14)	0.0301 (16)	0.0203 (15)
C10	0.0429 (15)	0.0698 (19)	0.085 (2)	0.0051 (13)	0.0267 (15)	0.0200 (16)
C11	0.0365 (13)	0.0570 (16)	0.0650 (17)	0.0033 (12)	0.0200 (12)	0.0083 (14)
C12	0.0465 (16)	0.0534 (16)	0.082 (2)	0.0024 (13)	0.0152 (15)	0.0128 (15)
C13	0.092 (2)	0.075 (2)	0.075 (2)	−0.016 (2)	0.0035 (19)	0.0106 (18)
C14	0.080 (2)	0.059 (2)	0.068 (2)	−0.0005 (17)	0.0083 (17)	0.0073 (17)
C15	0.117 (3)	0.073 (2)	0.090 (3)	0.010 (2)	0.032 (2)	0.013 (2)
C16	0.140 (4)	0.068 (3)	0.107 (3)	0.013 (2)	0.027 (3)	0.016 (2)
C17	0.133 (4)	0.089 (3)	0.092 (3)	−0.004 (3)	0.018 (3)	0.034 (2)
C18	0.153 (4)	0.126 (4)	0.097 (3)	0.015 (3)	0.060 (3)	0.023 (3)
C19	0.159 (4)	0.084 (3)	0.096 (3)	0.026 (3)	0.045 (3)	0.012 (2)
N1	0.0339 (12)	0.0570 (14)	0.0766 (17)	0.0029 (11)	0.0212 (11)	0.0144 (12)
O1	0.0800 (15)	0.0640 (13)	0.0849 (15)	0.0187 (12)	0.0356 (12)	0.0125 (12)
O2	0.0422 (11)	0.0794 (14)	0.1325 (19)	0.0128 (10)	0.0457 (12)	0.0399 (13)

Geometric parameters (Å, º)

C1—C2	1.511 (5)	C11—O2	1.234 (3)
C1—H1A	0.9600	C11—N1	1.321 (3)
C1—H1B	0.9600	C12—N1	1.441 (3)
C1—H1C	0.9600	C12—C13	1.483 (4)
C2—C7	1.389 (4)	C12—H12A	0.9700
C2—C3	1.396 (5)	C12—H12B	0.9700
C3—C4	1.369 (5)	C13—C14	1.504 (4)
C3—H3	0.9300	C13—H13A	0.9700
C4—C5	1.372 (4)	C13—H13B	0.9700
C4—H4	0.9300	C14—C15	1.352 (5)
C5—O1	1.375 (4)	C14—C19	1.377 (5)
C5—C6	1.387 (4)	C15—C16	1.380 (5)
C6—C7	1.386 (4)	C15—H15	0.9300

C6—C9	1.432 (4)	C16—C17	1.355 (6)
C7—H7	0.9300	C16—H16	0.9300
C8—C9	1.337 (4)	C17—C18	1.329 (6)
C8—O1	1.378 (3)	C17—H17	0.9300
C8—H8	0.9300	C18—C19	1.383 (6)
C9—C10	1.493 (4)	C18—H18	0.9300
C10—C11	1.505 (4)	C19—H19	0.9300
C10—H10A	0.9700	N1—H1	0.79 (3)
C10—H10B	0.9700		

C2—C1—H1A	109.5	O2—C11—C10	122.4 (2)
C2—C1—H1B	109.5	N1—C11—C10	115.9 (2)
H1A—C1—H1B	109.5	N1—C12—C13	114.3 (2)
C2—C1—H1C	109.5	N1—C12—H12A	108.7
H1A—C1—H1C	109.5	C13—C12—H12A	108.7
H1B—C1—H1C	109.5	N1—C12—H12B	108.7
C7—C2—C3	118.4 (4)	C13—C12—H12B	108.7
C7—C2—C1	121.0 (3)	H12A—C12—H12B	107.6
C3—C2—C1	120.6 (3)	C12—C13—C14	111.5 (3)
C4—C3—C2	123.0 (3)	C12—C13—H13A	109.3
C4—C3—H3	118.5	C14—C13—H13A	109.3
C2—C3—H3	118.5	C12—C13—H13B	109.3
C3—C4—C5	116.6 (3)	C14—C13—H13B	109.3
C3—C4—H4	121.7	H13A—C13—H13B	108.0
C5—C4—H4	121.7	C15—C14—C19	117.1 (3)
C4—C5—O1	126.3 (3)	C15—C14—C13	121.1 (3)
C4—C5—C6	123.5 (3)	C19—C14—C13	121.6 (3)
O1—C5—C6	110.2 (3)	C14—C15—C16	121.4 (4)
C7—C6—C5	118.3 (3)	C14—C15—H15	119.3
C7—C6—C9	135.4 (3)	C16—C15—H15	119.3
C5—C6—C9	106.2 (3)	C17—C16—C15	120.7 (4)
C6—C7—C2	120.2 (3)	C17—C16—H16	119.7
C6—C7—H7	119.9	C15—C16—H16	119.7
C2—C7—H7	119.9	C18—C17—C16	118.8 (4)
C9—C8—O1	112.9 (3)	C18—C17—H17	120.6
C9—C8—H8	123.5	C16—C17—H17	120.6
O1—C8—H8	123.5	C17—C18—C19	121.2 (4)
C8—C9—C6	105.8 (3)	C17—C18—H18	119.4
C8—C9—C10	127.2 (3)	C19—C18—H18	119.4
C6—C9—C10	127.0 (3)	C14—C19—C18	120.7 (4)
C9—C10—C11	114.2 (2)	C14—C19—H19	119.6
C9—C10—H10A	108.7	C18—C19—H19	119.6
C11—C10—H10A	108.7	C11—N1—C12	123.3 (2)
C9—C10—H10B	108.7	C11—N1—H1	113 (2)
C11—C10—H10B	108.7	C12—N1—H1	123 (2)
H10A—C10—H10B	107.6	C5—O1—C8	104.9 (2)
O2—C11—N1	121.6 (3)		

C7—C2—C3—C4	0.2 (5)	C6—C9—C10—C11	75.3 (4)
C1—C2—C3—C4	−179.6 (3)	C9—C10—C11—O2	−4.8 (4)
C2—C3—C4—C5	0.3 (5)	C9—C10—C11—N1	175.4 (3)
C3—C4—C5—O1	179.8 (3)	N1—C12—C13—C14	−170.0 (3)
C3—C4—C5—C6	−0.8 (5)	C12—C13—C14—C15	−73.6 (4)
C4—C5—C6—C7	0.9 (4)	C12—C13—C14—C19	101.9 (4)
O1—C5—C6—C7	−179.7 (2)	C19—C14—C15—C16	−0.9 (6)
C4—C5—C6—C9	−178.9 (3)	C13—C14—C15—C16	174.9 (3)
O1—C5—C6—C9	0.5 (3)	C14—C15—C16—C17	−0.4 (7)
C5—C6—C7—C2	−0.3 (4)	C15—C16—C17—C18	1.8 (7)
C9—C6—C7—C2	179.4 (3)	C16—C17—C18—C19	−1.9 (8)
C3—C2—C7—C6	−0.2 (4)	C15—C14—C19—C18	0.7 (6)
C1—C2—C7—C6	179.6 (3)	C13—C14—C19—C18	−175.0 (4)
O1—C8—C9—C6	−0.5 (3)	C17—C18—C19—C14	0.7 (8)
O1—C8—C9—C10	−177.4 (2)	O2—C11—N1—C12	2.5 (4)
C7—C6—C9—C8	−179.8 (3)	C10—C11—N1—C12	−177.7 (3)
C5—C6—C9—C8	0.0 (3)	C13—C12—N1—C11	123.3 (3)
C7—C6—C9—C10	−2.8 (5)	C4—C5—O1—C8	178.6 (3)
C5—C6—C9—C10	176.9 (3)	C6—C5—O1—C8	−0.8 (3)
C8—C9—C10—C11	−108.4 (3)	C9—C8—O1—C5	0.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.79 (3)	2.06 (3)	2.849 (3)	173 (3)

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