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N-(2-Methoxyphenyl)-2-nitrobenzamide

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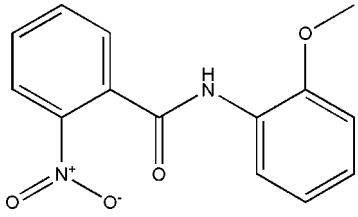
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.111; data-to-parameter ratio = 7.3.

Geometric parameters of the title compound, $C_{14}H_{12}N_2O_4$, are in the usual ranges. The dihedral angle between the two aromatic rings is 28.9 (1)°. The nitro group is twisted by 40.2 (1)° out of the plane of the aromatic ring to which it is attached. The crystal structure is stabilized by an N—H···O hydrogen bond.

Related literature

For related literature, see: Capdeville *et al.* (2002); Ho *et al.* (2002); Igawa *et al.* (1999); Jackson *et al.* (1994); Makino *et al.* (2001, 2003); Manley *et al.* (2002); Zhichkin *et al.* (2007).



Experimental

Crystal data

$C_{14}H_{12}N_2O_4$
M_r = 272.26
Orthorhombic, $P2_12_12_1$
a = 7.6467 (11) Å
b = 9.9272 (8) Å
c = 16.5032 (14) Å
V = 1252.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 173 (2) K
0.37 × 0.33 × 0.21 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
8342 measured reflections
1368 independent reflections
1275 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.110
S = 1.05
1368 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.82 (4)	2.57 (4)	3.352 (3)	159 (3)

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2111).

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N-(2-Methoxyphenyl)-2-nitrobenzamide

Aamer Saeed, Shahid Hussain and Michael Bolte

S1. Comment

The benzanilide core is present in compounds with such a wide range of biological activities that it has been called a privileged structure. Benzanilides serve as intermediates to benzothiadiazin-4-ones (Makino *et al.*, 2003), quinazoline-2,4-diones (Makino *et al.*, 2001), benzodiazepine-2,5-diones (Ho *et al.*, 2002) and 2,3-disubstituted 3*H*-quinazoline-4-ones (Zhichkin *et al.*, 2007). Benzanilides have established their efficacy as central elements of ligands that bind to a wide variety of receptor types. Thus a benzanilide containing aminoalkyl groups originally designed as a peptidomimetic has been incorporated in an Arg-Gly-Asp cyclic peptide yielding a high affinity GPIIb/IIIa ligand (Jackson *et al.*, 1994). Imatinib is an ATP-site binding kinase inhibitor and platelet-derived growth factor receptor kinases (Capdeville *et al.*, 2002). Pyridylmethyl containing benzanilides are vascular endothelial growth factor receptors and tyrosine kinase inhibitors (Manley *et al.*, 2002). Furthermore, benzamides have been reported to have activities as acetyl-CoA carboxylase and farnesyl transferase inhibitors (Igawa *et al.*, 1999)

Geometric parameters of the title compound, $C_{14}H_{12}N_2O_4$, are in the usual ranges. The dihedral angle between the two aromatic rings is 28.9 (1)°. The nitrogroup is twisted by 40.2 (1)° out of the plane of the phenyl ring to which it is attached. The crystal structure is stabilized by an N—H···O hydrogen bond.

S2. Experimental

A mixture of 2-methoxyaniline (10.0 g, 65.7 mmol), 2-nitrobenzoyl chloride (10 ml, 86.9 mmol), and pyridine (20 ml) was left at 25 °C for 15 h. Water (100 ml) was then added, and the resulting precipitate was collected. Recrystallization of the precipitate from benzene gave 12.6 g (75%) of the title compound as yellow blocks: mp 95–96 °C 1H NMR (CDCl3) δ 7.23–8.30 (m, 8H, Ar—Hs), 11.36 (br s, 1H, NH).

S3. Refinement

In the absence of anomalous scatterers, Friedel pairs had been merged and the absolute structure was arbitrarily assigned. All H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 U_{eq}(C_{methyl})] using a riding model with C—H = 0.95Å or C—H = 0.98Å for aromatic and methyl C, respectively. The methyl group was allowed to rotate, but not to tip. The amino H atom was freely refined.

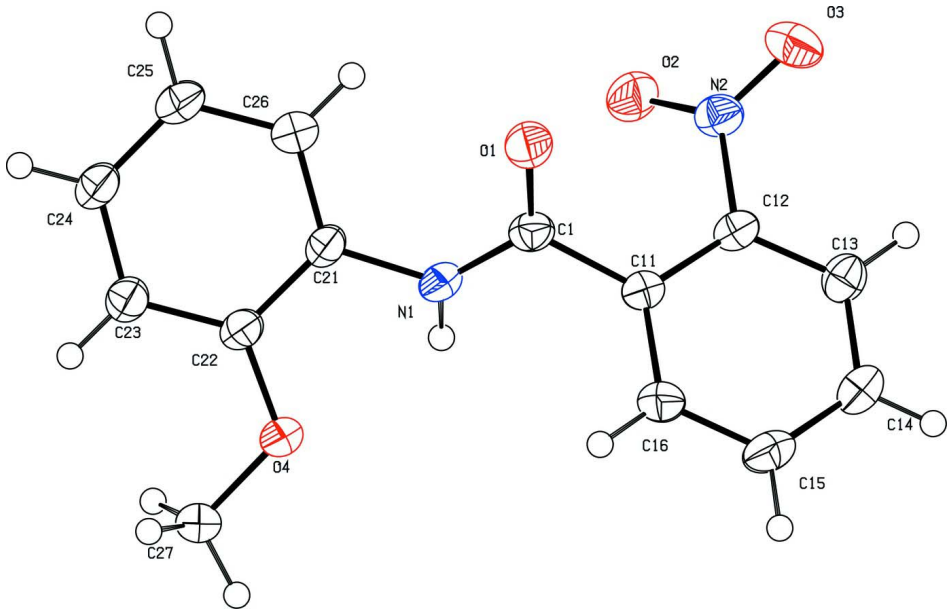

Figure 1

Molecular structure of the title compound.

N-(2-Methoxyphenyl)-2-nitrobenzamide

Crystal data

$C_{14}H_{12}N_2O_4$
$M_r = 272.26$
Orthorhombic, $P2_12_12_1$
$a = 7.6467$ (11) Å
$b = 9.9272$ (8) Å
$c = 16.5032$ (14) Å
$V = 1252.8$ (2) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.444$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7856 reflections
$\theta = 3.8$–25.6°
$\mu = 0.11$ mm^{-1}
$T = 173$ K
Block, light yellow
0.37 × 0.33 × 0.21 mm

Data collection

Stoe IPDSII two-circle diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
8342 measured reflections
1368 independent reflections
1275 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.6°$, $\theta_{min} = 3.6°$
$h = -7\rightarrow9$
$k = -12\rightarrow12$
$l = -20\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.110$
$S = 1.05$
1368 reflections
187 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

$w = 1/[\sigma^2(F_o^2) + (0.0824P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.052 (7)

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}
C1	0.7040 (3)	0.4189 (2)	0.58905 (15)	0.0271 (5)
N1	0.6935 (3)	0.46807 (19)	0.51339 (14)	0.0287 (5)
H1	0.618 (5)	0.449 (3)	0.4799 (19)	0.040 (9)*
N2	0.7600 (3)	0.14453 (18)	0.64422 (13)	0.0299 (5)
O1	0.8235 (3)	0.44489 (17)	0.63779 (11)	0.0370 (5)
O2	0.8450 (3)	0.16188 (18)	0.58190 (13)	0.0410 (5)
O3	0.8114 (3)	0.07915 (18)	0.70333 (13)	0.0419 (5)
O4	0.5752 (2)	0.62521 (16)	0.39737 (11)	0.0305 (5)
C11	0.5537 (3)	0.3307 (2)	0.61508 (14)	0.0263 (5)
C12	0.5833 (3)	0.2030 (2)	0.64870 (16)	0.0264 (5)
C13	0.4498 (4)	0.1261 (2)	0.68256 (15)	0.0307 (6)
H13	0.4744	0.0404	0.7055	0.037*
C14	0.2795 (4)	0.1764 (2)	0.68236 (17)	0.0338 (6)
H14	0.1869	0.1248	0.7049	0.041*
C15	0.2456 (4)	0.3028 (3)	0.64891 (17)	0.0360 (6)
H15	0.1294	0.3368	0.6483	0.043*
C16	0.3821 (4)	0.3800 (2)	0.61615 (17)	0.0324 (6)
H16	0.3579	0.4667	0.5945	0.039*
C21	0.8150 (3)	0.5560 (2)	0.47494 (14)	0.0260 (5)
C22	0.7505 (3)	0.6385 (2)	0.41263 (15)	0.0267 (5)
C23	0.8635 (4)	0.7254 (2)	0.37131 (16)	0.0293 (6)
H23	0.8199	0.7825	0.3297	0.035*
C24	1.0410 (4)	0.7277 (2)	0.39163 (16)	0.0314 (6)
H24	1.1177	0.7872	0.3638	0.038*
C25	1.1068 (4)	0.6440 (2)	0.45211 (17)	0.0323 (6)
H25	1.2280	0.6452	0.4649	0.039*
C26	0.9933 (4)	0.5579 (2)	0.49399 (15)	0.0299 (5)
H26	1.0374	0.5007	0.5354	0.036*
C27	0.5074 (4)	0.6982 (2)	0.32917 (16)	0.0323 (6)
H27A	0.5211	0.7951	0.3385	0.048*
H27B	0.3831	0.6769	0.3222	0.048*

H27C	0.5717	0.6724	0.2802	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0227 (13)	0.0256 (10)	0.0331 (13)	0.0022 (9)	−0.0009 (10)	−0.0013 (9)
N1	0.0195 (11)	0.0312 (10)	0.0354 (12)	−0.0040 (8)	−0.0015 (10)	0.0024 (8)
N2	0.0261 (12)	0.0246 (9)	0.0390 (12)	0.0014 (9)	−0.0020 (9)	−0.0034 (8)
O1	0.0324 (11)	0.0415 (9)	0.0372 (10)	−0.0095 (9)	−0.0085 (8)	0.0057 (8)
O2	0.0308 (11)	0.0429 (9)	0.0491 (11)	0.0067 (8)	0.0110 (9)	0.0029 (9)
O3	0.0413 (12)	0.0373 (8)	0.0470 (12)	0.0104 (9)	−0.0093 (9)	0.0037 (8)
O4	0.0209 (9)	0.0330 (8)	0.0374 (10)	−0.0019 (7)	−0.0012 (8)	0.0062 (7)
C11	0.0217 (12)	0.0282 (11)	0.0289 (12)	0.0003 (10)	−0.0005 (11)	0.0009 (9)
C12	0.0208 (14)	0.0269 (10)	0.0315 (12)	−0.0008 (9)	0.0007 (10)	−0.0038 (9)
C13	0.0312 (15)	0.0271 (10)	0.0338 (13)	−0.0040 (10)	0.0025 (12)	−0.0029 (9)
C14	0.0268 (15)	0.0368 (12)	0.0377 (14)	−0.0069 (11)	0.0047 (12)	−0.0027 (10)
C15	0.0216 (14)	0.0457 (13)	0.0408 (15)	0.0011 (11)	0.0024 (12)	−0.0023 (11)
C16	0.0255 (14)	0.0355 (12)	0.0362 (13)	0.0055 (10)	0.0001 (12)	0.0043 (10)
C21	0.0216 (12)	0.0247 (10)	0.0315 (12)	−0.0026 (10)	0.0041 (10)	0.0000 (9)
C22	0.0210 (12)	0.0261 (10)	0.0328 (12)	−0.0010 (9)	0.0016 (10)	−0.0011 (9)
C23	0.0270 (14)	0.0264 (10)	0.0345 (13)	−0.0007 (10)	0.0036 (11)	0.0005 (9)
C24	0.0247 (14)	0.0304 (11)	0.0390 (14)	−0.0047 (10)	0.0044 (12)	−0.0004 (10)
C25	0.0225 (13)	0.0345 (12)	0.0398 (13)	−0.0043 (11)	−0.0005 (11)	−0.0034 (10)
C26	0.0243 (13)	0.0328 (12)	0.0326 (12)	0.0005 (11)	−0.0010 (10)	−0.0008 (9)
C27	0.0240 (14)	0.0362 (12)	0.0367 (14)	0.0010 (10)	−0.0036 (11)	0.0074 (9)

Geometric parameters (Å, º)

C1—O1	1.244 (3)	C15—C16	1.404 (4)
C1—N1	1.343 (3)	C15—H15	0.9500
C1—C11	1.508 (3)	C16—H16	0.9500
N1—C21	1.424 (3)	C21—C26	1.399 (4)
N1—H1	0.82 (4)	C21—C22	1.404 (3)
N2—O2	1.229 (3)	C22—C23	1.399 (3)
N2—O3	1.236 (3)	C23—C24	1.399 (4)
N2—C12	1.473 (3)	C23—H23	0.9500
O4—C22	1.371 (3)	C24—C25	1.393 (4)
O4—C27	1.435 (3)	C24—H24	0.9500
C11—C16	1.400 (4)	C25—C26	1.401 (4)
C11—C12	1.402 (3)	C25—H25	0.9500
C12—C13	1.392 (4)	C26—H26	0.9500
C13—C14	1.395 (4)	C27—H27A	0.9800
C13—H13	0.9500	C27—H27B	0.9800
C14—C15	1.395 (4)	C27—H27C	0.9800
C14—H14	0.9500		
O1—C1—N1	124.7 (2)	C11—C16—H16	119.6
O1—C1—C11	119.7 (2)	C15—C16—H16	119.6

N1—C1—C11	115.5 (2)	C26—C21—C22	119.9 (2)
C1—N1—C21	126.7 (2)	C26—C21—N1	122.9 (2)
C1—N1—H1	126 (2)	C22—C21—N1	117.1 (2)
C21—N1—H1	107 (2)	O4—C22—C23	125.0 (2)
O2—N2—O3	124.5 (2)	O4—C22—C21	115.0 (2)
O2—N2—C12	118.2 (2)	C23—C22—C21	120.0 (2)
O3—N2—C12	117.3 (2)	C22—C23—C24	119.5 (2)
C22—O4—C27	116.69 (19)	C22—C23—H23	120.2
C16—C11—C12	117.5 (2)	C24—C23—H23	120.2
C16—C11—C1	121.0 (2)	C25—C24—C23	120.8 (2)
C12—C11—C1	121.0 (2)	C25—C24—H24	119.6
C13—C12—C11	122.5 (2)	C23—C24—H24	119.6
C13—C12—N2	118.5 (2)	C24—C25—C26	119.6 (3)
C11—C12—N2	119.0 (2)	C24—C25—H25	120.2
C12—C13—C14	119.1 (2)	C26—C25—H25	120.2
C12—C13—H13	120.4	C21—C26—C25	120.1 (2)
C14—C13—H13	120.4	C21—C26—H26	120.0
C13—C14—C15	119.8 (2)	C25—C26—H26	120.0
C13—C14—H14	120.1	O4—C27—H27A	109.5
C15—C14—H14	120.1	O4—C27—H27B	109.5
C14—C15—C16	120.3 (3)	H27A—C27—H27B	109.5
C14—C15—H15	119.8	O4—C27—H27C	109.5
C16—C15—H15	119.8	H27A—C27—H27C	109.5
C11—C16—C15	120.7 (2)	H27B—C27—H27C	109.5

O1—C1—N1—C21	0.8 (4)	C12—C11—C16—C15	−0.8 (4)
C11—C1—N1—C21	178.3 (2)	C1—C11—C16—C15	−172.8 (2)
O1—C1—C11—C16	118.2 (3)	C14—C15—C16—C11	1.2 (4)
N1—C1—C11—C16	−59.5 (3)	C1—N1—C21—C26	29.1 (4)
O1—C1—C11—C12	−53.6 (3)	C1—N1—C21—C22	−154.1 (2)
N1—C1—C11—C12	128.8 (2)	C27—O4—C22—C23	5.6 (3)
C16—C11—C12—C13	−0.2 (4)	C27—O4—C22—C21	−174.3 (2)
C1—C11—C12—C13	171.8 (2)	C26—C21—C22—O4	177.9 (2)
C16—C11—C12—N2	176.4 (2)	N1—C21—C22—O4	1.0 (3)
C1—C11—C12—N2	−11.6 (3)	C26—C21—C22—C23	−2.0 (3)
O2—N2—C12—C13	138.0 (3)	N1—C21—C22—C23	−178.8 (2)
O3—N2—C12—C13	−40.8 (3)	O4—C22—C23—C24	−178.8 (2)
O2—N2—C12—C11	−38.8 (3)	C21—C22—C23—C24	1.1 (4)
O3—N2—C12—C11	142.4 (2)	C22—C23—C24—C25	0.4 (4)
C11—C12—C13—C14	0.8 (4)	C23—C24—C25—C26	−1.0 (4)
N2—C12—C13—C14	−175.8 (2)	C22—C21—C26—C25	1.3 (4)
C12—C13—C14—C15	−0.4 (4)	N1—C21—C26—C25	178.0 (2)
C13—C14—C15—C16	−0.6 (4)	C24—C25—C26—C21	0.1 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N1—H1···O2^{i}	0.82 (4)	2.57 (4)	3.352 (3)	159 (3)

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