organic compounds

4-Bromo-N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)-benzenesulfonamide

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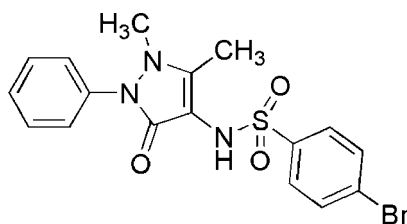
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In the title compound, $C_{17}H_{16}BrN_3O_3S$, the C—N—S—C torsion angle between the pyrazole unit and the bromobenzene ring is -117.3 (3)°. The phenyl ring and the pyrazole residue are twisted with respect to each other by an angle of 70.8 (2)°. One intermolecular N—H···O and two non-classical intermolecular C—H···O hydrogen bonds are observed in the crystal structure.

Related literature

For related literature, see: Cunha et al. (2005); Drew (2000); Kecskemeti et al. (2002); Petersen (2004); Prasad & Agarwal (2007); Supuran et al. (1996, 2003); Xue et al. (2000).

Experimental

Crystal data

$C_{17}H_{16}BrN_3O_3S$
$M_r = 422.30$
Orthorhombic, $P2_12_12_1$
$a = 7.979$ (1) Å
$b = 14.099$ (2) Å
$c = 15.685$ (3) Å

$V = 1764.5$ (5) Å^3
$Z = 4$
Cu $K\alpha$ radiation
$\mu = 4.47$ mm^{-1}
$T = 299$ (2) K
$0.60 \times 0.10 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North et al., 1968)
$T_{min} = 0.174$, $T_{max} = 0.663$
3508 measured reflections

3143 independent reflections
2998 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
3 standard reflections
  frequency: 120 min
  intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.120$
$S = 1.12$
3143 reflections
230 parameters
H-atom parameters constrained

$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.86$ e Å^{-3}
Absolute structure: Flack (1983), 1325 Friedel pairs
Flack parameter: -0.01 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O3^i	0.86	1.97	2.735 (4)	148
C5—H5···O1^{ii}	0.93	2.34	3.236 (5)	162
C11—H11···O1^{iii}	0.93	2.54	3.362 (6)	148

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

Data collection: CAD-4 PC-Software (Enraf–Nonius, 1996); cell refinement: CAD-4 PC-Software; data reduction: REDU4 (Stoe & Cie, 1987); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2074).

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supplementary materials

4-Bromo-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)benzenesulfonamide

L. E. da Silva, P. T. de Sousa Jr, E. N. Maciel, S. Foro and E. L. Dall'Oglio

Comment

4-aminoantipyrine derivatives are remarkable reagents due to theirs importance in biological, pharmacological, clinical and analytical applications (Cunha *et al.*, 2005; Prasad & Agarwal, 2007). On the other hand, sulfonamide is a pharmacophoric group of over than 30 pharmaceuticals which are in clinical use, with antibacterial (Drew, 2000), diuretic (Supuran *et al.*, 1996), oral antidiabetic (Kecskemeti *et al.*, 2002), antimalarial (Petersen, 2004), and HIV protease inhibitory (Supuran *et al.*, 2003) activities. In order to advance our extensive investigations about the chemical and biological aspects of sulfonamides, we have now synthesized different compounds of related structures, and we report here an X-ray crystallographic study of the title compound, (I).

The pyrazole moiety forms a C7—N1—S1—C1 dihedral angle with the bromobenzene ring of −117.3 (3)° and a dihedral angle between the mean planes of 70.8 (2)° with the phenyl ring indicating non-planarity in the molecule. The NH group has an intermolecular hydrogen bond to O3 [N—H⋯O = 1.97 Å]. C5 and C11 have an intermolecular contact to the sulfonyl oxygen atom O1 [C—H⋯O = 2.34 Å, C—H⋯O = 2.54 Å, respectively] (Table 1).

Experimental

Compound (I) was prepared according to a literature procedure (Xue *et al.*, 2000). Suitable crystals were obtained by re-crystallization from methanol-dichloromethane (1:1).

Refinement

The H atoms were positioned with idealized geometry using a riding model with N—H = 0.86 Å, C—H in the range 0.93–0.96 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom). The absolute structure was determined on the basis of 1325 Friedel pairs.
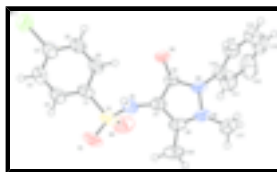
Figures

Fig. 1. Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

4-Bromo-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*- pyrazol-4-yl)benzenesulfonamide

Crystal data

C$_{17}$H$_{16}$BrN$_3$O$_3$S $F_{000} = 856$

supplementary materials

$M_r = 422.30$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 7.979 (1)$ Å

$b = 14.099 (2)$ Å

$c = 15.685 (3)$ Å

$V = 1764.5 (5)$ Å^3

$Z = 4$

$D_x = 1.590$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.54180$ Å

Cell parameters from 25 reflections

$\theta = 4.2$–$19.1°$

$\mu = 4.48$ mm^{-1}

$T = 299 (2)$ K

Needle, colorless

$0.60 \times 0.10 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 299(2)$ K

$\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{min} = 0.174$, $T_{max} = 0.663$

3508 measured reflections

3143 independent reflections

2998 reflections with $I > 2\sigma(I)$

$R_{int} = 0.059$

$\theta_{max} = 67.0°$

$\theta_{min} = 4.2°$

$h = -9 \rightarrow 0$

$k = -16 \rightarrow 0$

$l = -18 \rightarrow 18$

3 standard reflections

every 120 min

intensity decay: 1.0%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.120$

$S = 1.12$

3143 reflections

230 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.083P)^2 + 0.3533P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.010$

$\Delta\rho_{max} = 0.67$ e Å^{-3}

$\Delta\rho_{min} = -0.86$ e Å^{-3}

Extinction correction: SHELXL,
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0089 (7)

Absolute structure: Flack (1983), 1325 Friedel pairs

Flack parameter: −0.01 (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, convention-al 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 calculat-ing 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	0.6571 (4)	0.3881 (3)	0.3198 (2)	0.0488 (8)
C2	0.6266 (5)	0.4809 (3)	0.2954 (3)	0.0577 (9)
H2	0.5172	0.5006	0.2852	0.069*
C3	0.7550 (6)	0.5434 (3)	0.2860 (3)	0.0606 (9)
H3	0.7336	0.6058	0.2700	0.073*
C4	0.9168 (6)	0.5137 (3)	0.3006 (2)	0.0547 (9)
C5	0.9505 (5)	0.4220 (3)	0.3272 (3)	0.0576 (9)
H5	1.0601	0.4031	0.3381	0.069*
C6	0.8205 (5)	0.3593 (3)	0.3373 (3)	0.0554 (9)
H6	0.8414	0.2978	0.3558	0.066*
C7	0.5305 (4)	0.1624 (3)	0.4314 (2)	0.0463 (7)
C8	0.4135 (4)	0.0916 (3)	0.4305 (2)	0.0517 (8)
C9	0.6903 (4)	0.1207 (2)	0.4448 (2)	0.0427 (7)
C10	0.7795 (5)	−0.0495 (3)	0.4522 (2)	0.0470 (8)
C11	0.8040 (8)	−0.1022 (3)	0.3796 (3)	0.0764 (13)
H11	0.7424	−0.0893	0.3306	0.092*
C12	0.9195 (10)	−0.1736 (4)	0.3797 (4)	0.0928 (19)
H12	0.9362	−0.2096	0.3308	0.111*
C13	1.0108 (7)	−0.1925 (3)	0.4517 (4)	0.0833 (15)
H13	1.0906	−0.2406	0.4513	0.100*
C14	0.9850 (7)	−0.1414 (4)	0.5230 (4)	0.0802 (14)
H14	1.0450	−0.1554	0.5722	0.096*
C15	0.8692 (5)	−0.0678 (3)	0.5235 (3)	0.0605 (10)
H15	0.8536	−0.0315	0.5723	0.073*
C16	0.2263 (5)	0.1021 (4)	0.4269 (3)	0.0695 (12)
H16A	0.1983	0.1629	0.4033	0.083*
H16B	0.1810	0.0972	0.4834	0.083*
H16C	0.1800	0.0529	0.3917	0.083*
C17	0.4173 (7)	−0.0816 (4)	0.4623 (5)	0.0866 (16)
H17A	0.2976	−0.0783	0.4571	0.104*
H17B	0.4467	−0.0965	0.5201	0.104*
H17C	0.4597	−0.1300	0.4251	0.104*
Br1	1.09883 (7)	0.59820 (3)	0.28076 (4)	0.0729 (2)
N1	0.5009 (4)	0.2597 (2)	0.41965 (19)	0.0504 (7)
H1N	0.4871	0.2955	0.4635	0.086 (17)*
N2	0.4888 (4)	0.0077 (2)	0.4394 (2)	0.0542 (7)
N3	0.6597 (3)	0.0254 (2)	0.4524 (2)	0.0527 (8)
O1	0.3412 (4)	0.3610 (3)	0.3189 (3)	0.0821 (11)
O2	0.5239 (5)	0.2327 (3)	0.26507 (19)	0.0785 (9)
O3	0.8354 (3)	0.15550 (18)	0.44804 (18)	0.0501 (6)

S1	0.49208 (11)	0.30563 (8)	0.32547 (6)	0.0560 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0339 (16)	0.065 (2)	0.0473 (16)	0.0115 (15)	−0.0006 (13)	−0.0002 (16)
C2	0.045 (2)	0.066 (2)	0.062 (2)	0.0187 (17)	0.0000 (16)	0.0055 (18)
C3	0.067 (2)	0.052 (2)	0.063 (2)	0.0145 (18)	0.0025 (19)	0.0076 (19)
C4	0.055 (2)	0.059 (2)	0.0500 (18)	0.0120 (18)	0.0025 (16)	0.0015 (15)
C5	0.0387 (18)	0.063 (2)	0.071 (2)	0.0113 (15)	0.0016 (17)	0.0087 (19)
C6	0.0413 (19)	0.059 (2)	0.066 (2)	0.0113 (16)	0.0027 (17)	0.0103 (17)
C7	0.0337 (15)	0.0549 (19)	0.0503 (17)	0.0036 (14)	0.0017 (14)	−0.0043 (15)
C8	0.0281 (15)	0.073 (2)	0.0536 (17)	−0.0039 (18)	0.0015 (14)	−0.0070 (17)
C9	0.0299 (14)	0.0506 (18)	0.0477 (17)	0.0003 (13)	−0.0035 (14)	−0.0044 (13)
C10	0.0415 (17)	0.0432 (18)	0.0562 (18)	−0.0048 (14)	0.0012 (15)	0.0010 (15)
C11	0.104 (4)	0.063 (2)	0.062 (2)	0.009 (3)	−0.001 (3)	−0.007 (2)
C12	0.130 (5)	0.059 (3)	0.090 (3)	0.025 (3)	0.028 (4)	−0.008 (2)
C13	0.065 (3)	0.049 (2)	0.135 (5)	0.008 (2)	0.021 (3)	0.008 (3)
C14	0.056 (3)	0.072 (3)	0.112 (4)	0.004 (2)	−0.023 (3)	0.010 (3)
C15	0.048 (2)	0.067 (2)	0.066 (2)	0.0029 (17)	−0.0087 (18)	−0.0042 (18)
C16	0.0272 (16)	0.104 (3)	0.078 (3)	−0.002 (2)	0.0035 (16)	−0.011 (3)
C17	0.058 (3)	0.074 (3)	0.128 (5)	−0.024 (3)	−0.010 (3)	0.013 (3)
Br1	0.0682 (3)	0.0618 (3)	0.0889 (4)	−0.0030 (2)	0.0075 (3)	0.0051 (2)
N1	0.0413 (15)	0.0582 (17)	0.0516 (15)	0.0117 (14)	0.0027 (13)	−0.0016 (13)
N2	0.0287 (13)	0.0602 (18)	0.0737 (19)	−0.0093 (14)	−0.0022 (14)	−0.0029 (15)
N3	0.0276 (13)	0.0511 (16)	0.079 (2)	−0.0010 (12)	−0.0106 (14)	−0.0056 (15)
O1	0.0323 (14)	0.108 (3)	0.106 (3)	0.0158 (15)	−0.0135 (15)	0.030 (2)
O2	0.082 (2)	0.097 (2)	0.0563 (15)	−0.017 (2)	−0.0052 (16)	−0.0119 (15)
O3	0.0295 (11)	0.0522 (13)	0.0688 (15)	−0.0034 (10)	−0.0087 (11)	−0.0064 (11)
S1	0.0375 (4)	0.0765 (6)	0.0541 (5)	0.0055 (4)	−0.0080 (4)	0.0028 (4)

Geometric parameters (Å, °)

C1—C2	1.385 (6)	C11—C12	1.365 (8)
C1—C6	1.393 (5)	C11—H11	0.9300
C1—S1	1.759 (4)	C12—C13	1.370 (10)
C2—C3	1.360 (6)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.346 (8)
C3—C4	1.377 (6)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.389 (7)
C4—C5	1.385 (6)	C14—H14	0.9300
C4—Br1	1.903 (5)	C15—H15	0.9300
C5—C6	1.372 (6)	C16—H16A	0.9600
C5—H5	0.9300	C16—H16B	0.9600
C6—H6	0.9300	C16—H16C	0.9600
C7—C8	1.366 (5)	C17—N2	1.428 (6)
C7—N1	1.404 (5)	C17—H17A	0.9600
C7—C9	1.420 (5)	C17—H17B	0.9600
C8—N2	1.335 (5)	C17—H17C	0.9600

C8—C16	1.502 (5)	N1—S1	1.614 (3)
C9—O3	1.259 (4)	N1—H1N	0.8600
C9—N3	1.370 (5)	N2—N3	1.402 (4)
C10—C15	1.353 (6)	O1—S1	1.439 (3)
C10—C11	1.374 (6)	O2—S1	1.421 (4)
C10—N3	1.424 (5)		
C2—C1—C6	119.6 (4)	C14—C13—C12	119.9 (5)
C2—C1—S1	120.5 (3)	C14—C13—H13	120.0
C6—C1—S1	119.9 (3)	C12—C13—H13	120.0
C3—C2—C1	120.7 (4)	C13—C14—C15	120.4 (5)
C3—C2—H2	119.7	C13—C14—H14	119.8
C1—C2—H2	119.7	C15—C14—H14	119.8
C2—C3—C4	119.5 (4)	C10—C15—C14	119.3 (4)
C2—C3—H3	120.3	C10—C15—H15	120.3
C4—C3—H3	120.3	C14—C15—H15	120.3
C3—C4—C5	121.0 (4)	C8—C16—H16A	109.5
C3—C4—Br1	119.9 (3)	C8—C16—H16B	109.5
C5—C4—Br1	119.0 (3)	H16A—C16—H16B	109.5
C6—C5—C4	119.3 (4)	C8—C16—H16C	109.5
C6—C5—H5	120.3	H16A—C16—H16C	109.5
C4—C5—H5	120.3	H16B—C16—H16C	109.5
C5—C6—C1	119.8 (4)	N2—C17—H17A	109.5
C5—C6—H6	120.1	N2—C17—H17B	109.5
C1—C6—H6	120.1	H17A—C17—H17B	109.5
C8—C7—N1	126.7 (4)	N2—C17—H17C	109.5
C8—C7—C9	108.2 (3)	H17A—C17—H17C	109.5
N1—C7—C9	125.1 (3)	H17B—C17—H17C	109.5
N2—C8—C7	109.8 (3)	C7—N1—S1	121.3 (3)
N2—C8—C16	122.6 (4)	C7—N1—H1N	119.4
C7—C8—C16	127.4 (5)	S1—N1—H1N	119.4
O3—C9—N3	122.9 (3)	C8—N2—N3	107.1 (3)
O3—C9—C7	132.1 (3)	C8—N2—C17	128.9 (4)
N3—C9—C7	105.0 (3)	N3—N2—C17	120.6 (4)
C15—C10—C11	120.4 (4)	C9—N3—N2	109.6 (3)
C15—C10—N3	119.6 (4)	C9—N3—C10	127.4 (3)
C11—C10—N3	119.9 (4)	N2—N3—C10	121.3 (3)
C12—C11—C10	119.6 (5)	O2—S1—O1	119.6 (3)
C12—C11—H11	120.2	O2—S1—N1	108.18 (19)
C10—C11—H11	120.2	O1—S1—N1	108.63 (19)
C11—C12—C13	120.3 (5)	O2—S1—C1	108.1 (2)
C11—C12—H12	119.9	O1—S1—C1	105.3 (2)
C13—C12—H12	119.9	N1—S1—C1	106.19 (18)
C6—C1—C2—C3	1.8 (6)	C9—C7—N1—S1	93.4 (4)
S1—C1—C2—C3	−176.1 (3)	C7—C8—N2—N3	4.1 (4)
C1—C2—C3—C4	0.4 (6)	C16—C8—N2—N3	−171.7 (4)
C2—C3—C4—C5	−2.1 (6)	C7—C8—N2—C17	163.3 (5)
C2—C3—C4—Br1	176.0 (3)	C16—C8—N2—C17	−12.6 (7)
C3—C4—C5—C6	1.5 (6)	O3—C9—N3—N2	−175.3 (3)

Br1—C4—C5—C6	−176.6 (3)	C7—C9—N3—N2	3.3 (4)
C4—C5—C6—C1	0.8 (6)	O3—C9—N3—C10	−10.1 (6)
C2—C1—C6—C5	−2.4 (6)	C7—C9—N3—C10	168.5 (4)
S1—C1—C6—C5	175.5 (3)	C8—N2—N3—C9	−4.7 (4)
N1—C7—C8—N2	176.8 (3)	C17—N2—N3—C9	−165.9 (4)
C9—C7—C8—N2	−2.1 (4)	C8—N2—N3—C10	−170.9 (3)
N1—C7—C8—C16	−7.6 (7)	C17—N2—N3—C10	27.9 (6)
C9—C7—C8—C16	173.5 (4)	C15—C10—N3—C9	78.7 (5)
C8—C7—C9—O3	177.6 (4)	C11—C10—N3—C9	−100.8 (5)
N1—C7—C9—O3	−1.3 (6)	C15—C10—N3—N2	−117.7 (4)
C8—C7—C9—N3	−0.8 (4)	C11—C10—N3—N2	62.8 (5)
N1—C7—C9—N3	−179.7 (3)	C7—N1—S1—O2	−1.8 (4)
C15—C10—C11—C12	0.2 (8)	C7—N1—S1—O1	129.4 (3)
N3—C10—C11—C12	179.7 (5)	C7—N1—S1—C1	−117.7 (3)
C10—C11—C12—C13	−0.2 (9)	C2—C1—S1—O2	117.0 (3)
C11—C12—C13—C14	1.0 (9)	C6—C1—S1—O2	−60.8 (4)
C12—C13—C14—C15	−1.7 (8)	C2—C1—S1—O1	−11.9 (4)
C11—C10—C15—C14	−0.9 (7)	C6—C1—S1—O1	170.2 (3)
N3—C10—C15—C14	179.6 (4)	C2—C1—S1—N1	−127.0 (3)
C13—C14—C15—C10	1.7 (8)	C6—C1—S1—N1	55.1 (4)
C8—C7—N1—S1	−85.3 (5)		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O3[i]	0.86	1.97	2.735 (4)	148
C5—H5···O1[ii]	0.93	2.34	3.236 (5)	162
C11—H11···O1[iii]	0.93	2.54	3.362 (6)	148

Symmetry codes: (i) $x-1/2$, $-y+1/2$, $-z+1$; (ii) $x+1$, y, z; (iii) $-x+1$, $y-1/2$, $-z+1/2$.

Fig. 1