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(*R*)-1-(4-Bromobenzoyl)-4-(1-phenylpropyl)thiosemicarbazide

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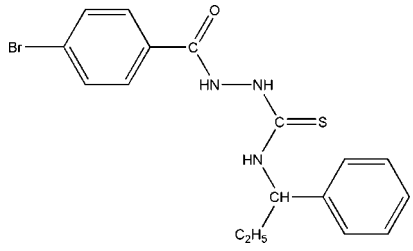
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.074; data-to-parameter ratio = 17.5.

The title compound, $C_{17}H_{18}BrN_3OS$, is an important intermediate for the synthesis of biologically active heterocyclic compounds. The thiourea group is approximately planar. The crystal structure is stabilized by intermolecular N—H···O hydrogen-bonding interactions.

Related literature

For related literature, see: Akhtar *et al.* (2006, 2007); Cardia *et al.* (2006); Dolman *et al.* (2006); Hassan *et al.* (2006); Jalilian *et al.* (2000); Kucukguzel *et al.* (2006); Mohareb *et al.* (2007); Singh *et al.* (2003, 2005).



Experimental

Crystal data

$C_{17}H_{18}BrN_3OS$
M_r = 392.31
Orthorhombic, $P2_12_12_1$
a = 6.263 (3) Å
b = 9.698 (5) Å
c = 27.651 (15) Å
V = 1679.5 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.58 mm^{-1}
T = 123 (2) K
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: integration (*NUMABS*; Higashi, 1999)
T_{min} = 0.512, T_{max} = 0.626
13732 measured reflections
3824 independent reflections
3516 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.074
S = 1.13
3824 reflections
219 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), 1584 Friedel pairs
Flack parameter: 0.020 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.84 (4)	2.03 (4)	2.834 (4)	161 (4)

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2385).

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supporting information

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(*R*)-1-(4-Bromobenzoyl)-4-(1-phenylpropyl)thiosemicarbazide

Monazza Serwer, M. Khawar Rauf, Masahiro Ebihara and Shahid Hameed

S1. Comment

Thiosemicarbazides have attracted much attention partly because of their biological activities such as antifungal (Mohareb *et al.*, 2007), antibacterial (Kucukguzel *et al.*, 2006), antiamoebic (Singh *et al.*, 2005) antitubercular (Cardia *et al.*,2006), corrosion inhibitors (Singh *et al.*, 2003) and partly because of their use as intermediates in the synthesis of many biologically active heterocyclic compounds like 1,3,4-oxadiazoles (Dolman *et al.*, 2006), 1,3,4-thiadiazoles (Jalilian *et al.*,2000) and 1,2,4-triazole (Akhtar *et al.*, 2007; Akhtar *et al.*, 2006). The other important biologically active compounds synthesized from thiosemicarbazides include thiazoles, thiazines, thiadiazines, pyrazines and indazoles (Hassan *et al.*, 2006). The C2—S1 and C1—O1 bonds both show the expected full double-bond character, while the short values for the C1—N1, C2—N2, N1—N2,C2—N3 and C9—N3 bond lengths also indicate partial double-bond character. The thiourea group is approximately planar. The crystal packing is stabilized by N(1)—H(1)···O(1) and N(3)—H(3)···S(1) hydrogen bonds.

S2. Experimental

The 4-bromobenzoic acid hydrazide (0.0068 moles) was dissolved in methanol (30ml) and a solution of 0.0066 moles of R-(+)-1-phenylpropylisothiocyanate, separately dissolved in 10 ml of methanol, was added drop wise with continuous stirring. The reaction mixture was refluxed and after consumption of the starting materials (tlc), the mixture was cooled to room temperature and methanol evaporated in vacuo. The crude thiosemicarbazide was recrystallized from a mixture of ethyl acetate and petroleum ether. Yield: 85%; m.p 160-161 °C; R_f: 0.34 (Petroleum ether: acetone; 6:4); IR (ν_{max}, KBr, cm^{-1}): 3378, 3273, 3191, 3033, 2967, 2877, 1669, 1238, 1591, 1528, 699; ^{1}H-NMR (Acetone-d_6): δ 9.81 (1H, s), 8.58 (1H, s), 8.06 (1H, s), 0.97 (3H, t, J = 7.5 Hz), 1.92-1.82 (2H, m), 5.58 (1H, dd, J = 15.6, 7.2 Hz), 7.39 (2H, dd, J = 7.2, 1.5 Hz), 7.30 (2H, dt, J = 7.5, 3.0 Hz), 7.22 (1H, dt, J = 7.2, 3.0 Hz), 7.92 (2H, d, J = 8.4 Hz), 7.72 (2H, d, J = 8.7 Hz); ^{13}C-NMR (Acetone-d_6):δ 183.51, 165.60, 142.88, 133.20, 131.64, 129.61, 128.10, 126.87, 126.74,126.12, 59.55, 28.21, 10.47; EIMS: (m/z %) 214 (20), 183 (100), 155 (55),104 (10), 76 (50), 50 (45). Elemental analysis for $C_{17}H_{18}N_3SOBr$ (391):C, 52.05; H, 4.62; N, 10.71; S, 8.17. Found: C, 51.96; H, 4.70; N, 10.82; S, 8.07.

S3. Refinement

H atom on the N atom was refined isotropically. Other H atoms were placed in idealized positions and treated as riding atoms with C—H distance in the range 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

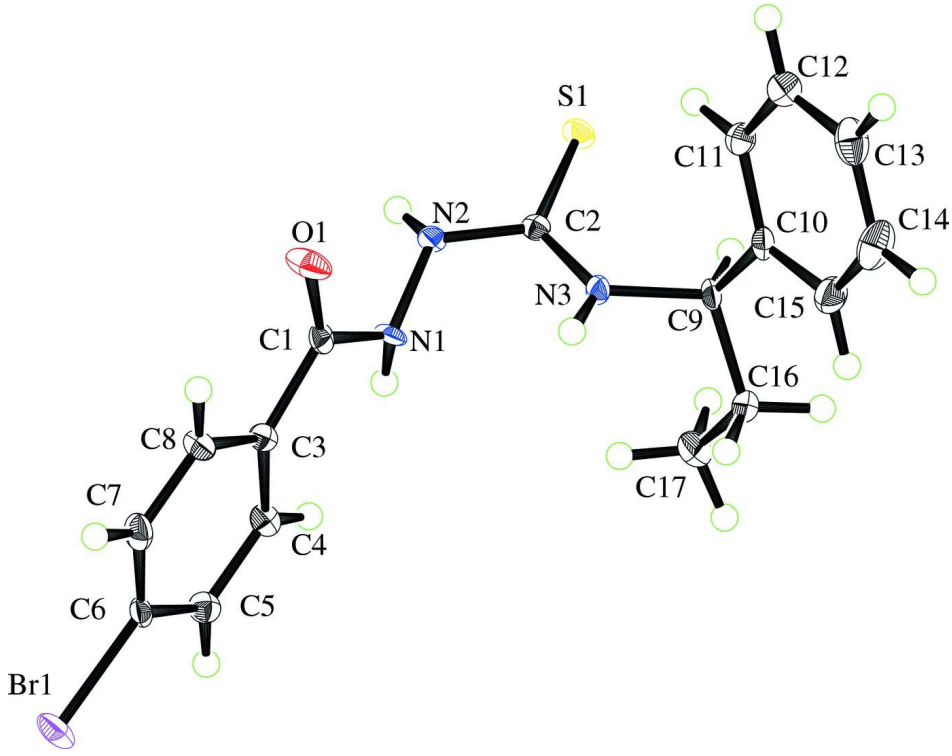

Figure 1

Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 30% probability level.

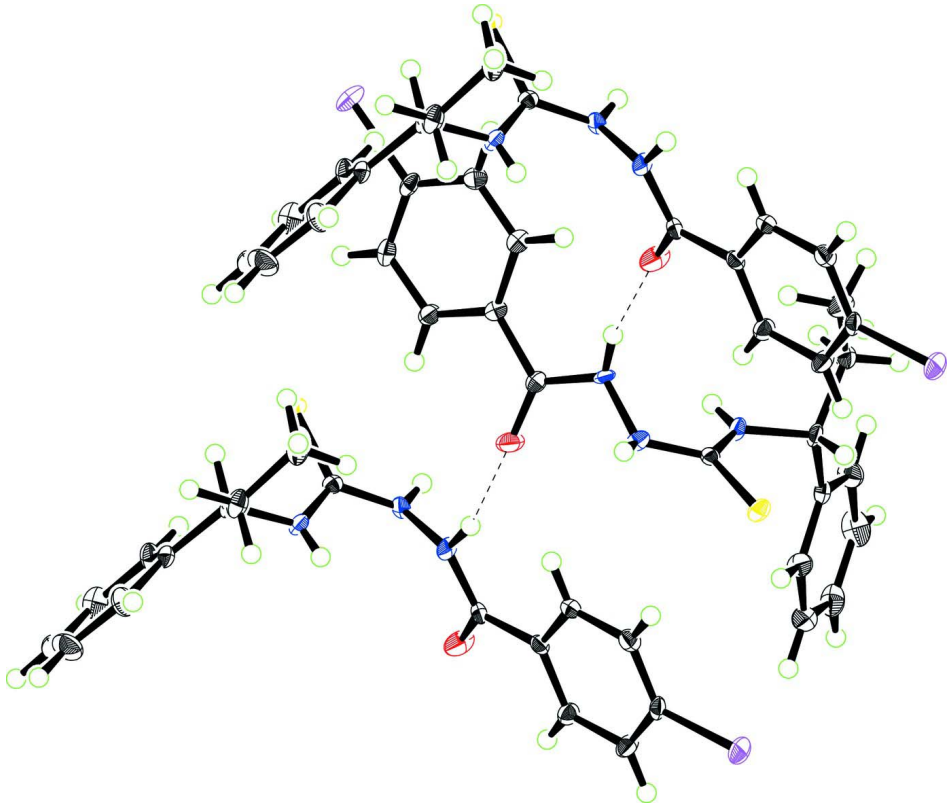

Figure 2

Showing hydrogen bonded molecules through N—H···O.

(*R*)-1-(4-Bromobenzoyl)-4-(1-phenylpropyl)thiosemicarbazide

Crystal data

$C_{17}H_{18}BrN_3OS$
$M_r = 392.31$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.263$ (3) Å
$b = 9.698$ (5) Å
$c = 27.651$ (15) Å
$V = 1679.5$ (15) Å^3
$Z = 4$
$F(000) = 800$
$D_x = 1.552$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 4820 reflections
$\theta = 3.1$–$27.5°$
$\mu = 2.58$ mm^{-1}
$T = 123$ K
Block, colourles
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: integration (*NUMABS*; Higashi, 1999)
$T_{min} = 0.512$, $T_{max} = 0.627$
13732 measured reflections
3824 independent reflections
3516 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -8 \rightarrow 8$
$k = -12 \rightarrow 8$
$l = -26 \rightarrow 35$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.074$
$S = 1.13$
3824 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + 1.3691P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0018 (4)
Absolute structure: Flack (1983), 1584 Friedel pairs
Absolute structure parameter: 0.020 (10)

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	0.0742 (6)	0.2098 (3)	0.24009 (12)	0.0141 (8)
O1	0.0089 (4)	0.0922 (2)	0.23367 (10)	0.0260 (7)
N1	−0.0306 (5)	0.3005 (3)	0.26956 (12)	0.0144 (7)
H1	0.006 (6)	0.384 (4)	0.2666 (13)	0.017*
C2	−0.2924 (6)	0.2804 (3)	0.33209 (13)	0.0124 (8)
S1	−0.55059 (15)	0.30911 (9)	0.34643 (4)	0.0169 (2)
N2	−0.2383 (5)	0.2701 (3)	0.28467 (12)	0.0144 (7)
H2	−0.319 (7)	0.288 (4)	0.2668 (15)	0.017*
N3	−0.1369 (5)	0.2639 (3)	0.36436 (12)	0.0146 (6)
H3	−0.024 (6)	0.254 (3)	0.3547 (15)	0.017*
C3	0.2725 (6)	0.2613 (3)	0.21649 (13)	0.0134 (8)
C4	0.3408 (6)	0.3985 (4)	0.21787 (13)	0.0156 (8)
H4	0.2625	0.4643	0.2361	0.019*
C5	0.5216 (6)	0.4390 (3)	0.19285 (14)	0.0171 (8)
H5	0.5681	0.5322	0.1939	0.020*
C6	0.6334 (7)	0.3426 (3)	0.16636 (12)	0.0153 (7)
C7	0.5710 (6)	0.2056 (4)	0.16486 (13)	0.0197 (8)
H7	0.6508	0.1401	0.1468	0.024*
C8	0.3915 (7)	0.1659 (3)	0.18998 (13)	0.0169 (8)
H8	0.3479	0.0721	0.1893	0.020*
Br1	0.87772 (7)	0.39971 (4)	0.131114 (15)	0.02482 (12)
C9	−0.1593 (6)	0.2802 (3)	0.41665 (12)	0.0152 (8)

H9	−0.3033	0.3217	0.4224	0.018*
C10	−0.1581 (6)	0.1398 (3)	0.44199 (13)	0.0154 (8)
C11	−0.3136 (6)	0.0440 (3)	0.42905 (14)	0.0207 (9)
H11	−0.4171	0.0674	0.4053	0.025*
C12	−0.3188 (7)	−0.0852 (4)	0.45040 (15)	0.0258 (10)
H12	−0.4244	−0.1503	0.4410	0.031*
C13	−0.1711 (7)	−0.1193 (4)	0.48521 (14)	0.0273 (10)
H13	−0.1748	−0.2078	0.4999	0.033*
C14	−0.0166 (7)	−0.0245 (4)	0.49888 (16)	0.0305 (11)
H14	0.0848	−0.0475	0.5231	0.037*
C15	−0.0110 (6)	0.1039 (4)	0.47705 (14)	0.0231 (9)
H15	0.0956	0.1683	0.4863	0.028*
C16	0.0052 (6)	0.3842 (4)	0.43521 (13)	0.0200 (8)
H16A	0.1506	0.3475	0.4296	0.024*
H16B	−0.0137	0.3966	0.4705	0.024*
C17	−0.0165 (7)	0.5243 (4)	0.41003 (15)	0.0276 (10)
H17A	0.0209	0.5147	0.3758	0.041*
H17B	0.0798	0.5909	0.4254	0.041*
H17C	−0.1641	0.5569	0.4129	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.017 (2)	0.0147 (16)	0.0109 (19)	0.0004 (14)	0.0000 (16)	0.0045 (13)
O1	0.0226 (16)	0.0156 (12)	0.0397 (18)	−0.0052 (12)	0.0131 (13)	−0.0043 (12)
N1	0.0114 (16)	0.0133 (13)	0.0185 (19)	−0.0054 (12)	0.0049 (14)	0.0010 (12)
C2	0.0131 (19)	0.0096 (15)	0.015 (2)	−0.0006 (13)	0.0013 (16)	−0.0013 (13)
S1	0.0102 (5)	0.0220 (4)	0.0184 (5)	0.0014 (4)	0.0029 (4)	0.0007 (4)
N2	0.0078 (17)	0.0215 (16)	0.0140 (19)	−0.0001 (13)	−0.0027 (14)	0.0057 (13)
N3	0.0102 (15)	0.0230 (13)	0.0105 (16)	0.0013 (12)	0.0013 (17)	−0.0019 (12)
C3	0.0120 (19)	0.0140 (16)	0.014 (2)	0.0009 (13)	−0.0015 (16)	0.0044 (13)
C4	0.015 (2)	0.0156 (15)	0.0165 (19)	0.0032 (17)	0.0005 (16)	0.0038 (15)
C5	0.018 (2)	0.0155 (17)	0.018 (2)	−0.0002 (14)	−0.0004 (18)	0.0023 (14)
C6	0.0116 (18)	0.0256 (16)	0.0087 (18)	0.0002 (15)	0.0002 (18)	0.0040 (13)
C7	0.020 (2)	0.0242 (17)	0.015 (2)	0.0037 (15)	0.0044 (17)	−0.0027 (15)
C8	0.016 (2)	0.0158 (15)	0.019 (2)	−0.0009 (15)	0.0043 (19)	0.0004 (13)
Br1	0.01688 (19)	0.03197 (19)	0.0256 (2)	−0.00092 (17)	0.0097 (2)	0.00672 (18)
C9	0.015 (2)	0.0230 (17)	0.0078 (19)	−0.0003 (15)	0.0031 (16)	−0.0007 (13)
C10	0.018 (2)	0.0194 (16)	0.0090 (18)	0.0018 (14)	0.0014 (17)	−0.0006 (12)
C11	0.020 (2)	0.0270 (18)	0.015 (2)	−0.0036 (15)	−0.0038 (17)	0.0045 (15)
C12	0.028 (3)	0.028 (2)	0.021 (2)	−0.0071 (18)	0.0013 (18)	−0.0019 (17)
C13	0.038 (3)	0.0230 (19)	0.021 (2)	0.0071 (18)	0.005 (2)	0.0009 (16)
C14	0.035 (3)	0.033 (2)	0.023 (3)	0.0116 (19)	−0.011 (2)	0.0005 (18)
C15	0.027 (2)	0.0242 (18)	0.018 (2)	−0.0021 (19)	−0.0045 (18)	0.0018 (18)
C16	0.020 (2)	0.0275 (18)	0.013 (2)	−0.0051 (16)	0.0007 (16)	−0.0030 (16)
C17	0.032 (3)	0.030 (2)	0.021 (2)	−0.0109 (18)	0.004 (2)	0.0027 (17)

Geometric parameters (Å, º)

C1—O1	1.224 (4)	C8—H8	0.9500
C1—N1	1.367 (4)	C9—C16	1.531 (5)
C1—C3	1.489 (5)	C9—C10	1.532 (4)
N1—N2	1.397 (4)	C9—H9	1.0000
N1—H1	0.84 (4)	C10—C15	1.382 (5)
C2—N3	1.330 (5)	C10—C11	1.393 (5)
C2—N2	1.358 (5)	C11—C12	1.386 (5)
C2—S1	1.688 (4)	C11—H11	0.9500
N2—H2	0.73 (4)	C12—C13	1.376 (6)
N3—C9	1.461 (5)	C12—H12	0.9500
N3—H3	0.76 (4)	C13—C14	1.387 (6)
C3—C8	1.396 (5)	C13—H13	0.9500
C3—C4	1.398 (5)	C14—C15	1.384 (5)
C4—C5	1.384 (5)	C14—H14	0.9500
C4—H4	0.9500	C15—H15	0.9500
C5—C6	1.379 (5)	C16—C17	1.532 (5)
C5—H5	0.9500	C16—H16A	0.9900
C6—C7	1.386 (5)	C16—H16B	0.9900
C6—Br1	1.897 (4)	C17—H17A	0.9800
C7—C8	1.376 (5)	C17—H17B	0.9800
C7—H7	0.9500	C17—H17C	0.9800
O1—C1—N1	121.7 (3)	C16—C9—C10	115.4 (3)
O1—C1—C3	121.8 (3)	N3—C9—H9	106.8
N1—C1—C3	116.5 (3)	C16—C9—H9	106.8
C1—N1—N2	119.3 (3)	C10—C9—H9	106.8
C1—N1—H1	115 (3)	C15—C10—C11	118.6 (3)
N2—N1—H1	119 (3)	C15—C10—C9	123.3 (3)
N3—C2—N2	117.1 (3)	C11—C10—C9	118.2 (3)
N3—C2—S1	124.3 (3)	C12—C11—C10	120.7 (4)
N2—C2—S1	118.6 (3)	C12—C11—H11	119.6
C2—N2—N1	120.4 (3)	C10—C11—H11	119.6
C2—N2—H2	118 (3)	C13—C12—C11	120.0 (4)
N1—N2—H2	113 (3)	C13—C12—H12	120.0
C2—N3—C9	125.5 (3)	C11—C12—H12	120.0
C2—N3—H3	117 (3)	C12—C13—C14	120.0 (4)
C9—N3—H3	117 (3)	C12—C13—H13	120.0
C8—C3—C4	118.8 (3)	C14—C13—H13	120.0
C8—C3—C1	117.0 (3)	C15—C14—C13	119.7 (4)
C4—C3—C1	124.2 (3)	C15—C14—H14	120.2
C5—C4—C3	120.4 (3)	C13—C14—H14	120.2
C5—C4—H4	119.8	C10—C15—C14	121.1 (4)
C3—C4—H4	119.8	C10—C15—H15	119.5
C6—C5—C4	119.2 (3)	C14—C15—H15	119.5
C6—C5—H5	120.4	C9—C16—C17	111.8 (3)
C4—C5—H5	120.4	C9—C16—H16A	109.3

C5—C6—C7	121.5 (4)	C17—C16—H16A	109.3
C5—C6—Br1	119.0 (3)	C9—C16—H16B	109.3
C7—C6—Br1	119.5 (3)	C17—C16—H16B	109.3
C8—C7—C6	118.9 (3)	H16A—C16—H16B	107.9
C8—C7—H7	120.5	C16—C17—H17A	109.5
C6—C7—H7	120.5	C16—C17—H17B	109.5
C7—C8—C3	121.0 (3)	H17A—C17—H17B	109.5
C7—C8—H8	119.5	C16—C17—H17C	109.5
C3—C8—H8	119.5	H17A—C17—H17C	109.5
N3—C9—C16	109.8 (3)	H17B—C17—H17C	109.5
N3—C9—C10	110.8 (3)		

O1—C1—N1—N2	−13.7 (5)	C4—C3—C8—C7	−1.1 (6)
C3—C1—N1—N2	166.7 (3)	C1—C3—C8—C7	176.6 (3)
N3—C2—N2—N1	−26.7 (4)	C2—N3—C9—C16	−125.2 (3)
S1—C2—N2—N1	154.7 (2)	C2—N3—C9—C10	106.1 (4)
C1—N1—N2—C2	131.2 (3)	N3—C9—C10—C15	121.4 (4)
N2—C2—N3—C9	175.6 (3)	C16—C9—C10—C15	−4.2 (5)
S1—C2—N3—C9	−6.0 (4)	N3—C9—C10—C11	−58.7 (4)
O1—C1—C3—C8	−5.4 (5)	C16—C9—C10—C11	175.7 (3)
N1—C1—C3—C8	174.2 (3)	C15—C10—C11—C12	−0.8 (6)
O1—C1—C3—C4	172.1 (3)	C9—C10—C11—C12	179.3 (3)
N1—C1—C3—C4	−8.3 (5)	C10—C11—C12—C13	0.8 (6)
C8—C3—C4—C5	0.8 (5)	C11—C12—C13—C14	−0.1 (6)
C1—C3—C4—C5	−176.7 (3)	C12—C13—C14—C15	−0.5 (6)
C3—C4—C5—C6	0.2 (5)	C11—C10—C15—C14	0.2 (6)
C4—C5—C6—C7	−1.1 (6)	C9—C10—C15—C14	−180.0 (4)
C4—C5—C6—Br1	178.7 (3)	C13—C14—C15—C10	0.5 (6)
C5—C6—C7—C8	0.8 (6)	N3—C9—C16—C17	57.4 (4)
Br1—C6—C7—C8	−179.0 (3)	C10—C9—C16—C17	−176.5 (3)
C6—C7—C8—C3	0.3 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.84 (4)	2.03 (4)	2.834 (4)	161 (4)

Symmetry code: (i) −*x*, *y*+1/2, −*z*+1/2.