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N-(Benzothiazol-2-yl)butyramide

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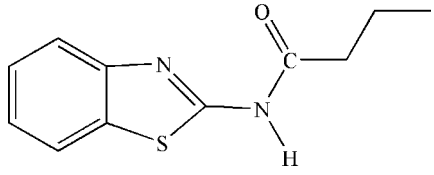
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.091; data-to-parameter ratio = 19.3.

The title compound, $C_{11}H_{12}N_2OS$, was synthesized from 2-aminobenzothiazole and butanoyl chloride in anhydrous acetone. In the crystal structure, molecules are linked by N—H···N and C—H···O hydrogen bonds and by C—H···π interactions.

Related literature

For related literature, see: Butt *et al.* (2005); Im & Jung (2000); Yang *et al.* (2002); Ataei *et al.* (2005).



Experimental

Crystal data

$C_{11}H_{12}N_2OS$
M_r = 220.29
Triclinic, $P\overline{1}$
a = 5.2916 (4) Å
b = 7.4462 (8) Å
c = 13.565 (1) Å
α = 92.618 (7)°
β = 90.607 (6)°
γ = 107.185 (8)°
V = 509.92 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 100 (2) K
0.35 × 0.20 × 0.05 mm

Data collection

Oxford Diffraction Xcalibur S diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
T_{min} = 0.977, T_{max} = 1.000 (expected range = 0.963–0.986)
8577 measured reflections
2728 independent reflections
2172 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 0.99
2728 reflections
141 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.84 (2)	2.40 (2)	3.232 (2)	172 (1)
C10—H10···O^{ii}	0.95	2.46	3.277 (2)	144
C2—H2B···$Cg1^{iii}$	0.99	2.66	3.56	152
C3—H3B···$Cg1^{iv}$	0.99	2.64	3.47	142

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y, -z+1$. $Cg1$ is the centroid of the C6–C11 ring.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to Allama Iqbal Open University, Islamabad, Pakistan, for providing the research and analytical laboratory facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2075).

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supporting information

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S1. Comment

High temperature polymers have received much attention due to the increasing demands for the replacement of ceramics and metals (Ataei *et al.*, 2005). However, in many cases, they are insoluble and do not melt below their decomposition temperature,which restricts their applications (Im & Jung, 2000). Thus, many studies have focused on obtaining aromatic polymers that are processable by conventional techniques (Yang *et al.*, 2002). The title compound, (I), is a precursor for an attempt to synthesize polyimides (Butt *et al.*, 2005), imidazole derivatives and transition metal complexes. The entire molecule (except H atoms) is planar within a mean deviation of 0.03 Å. Molecules are connected in ribbons parallel to [210] by classical hydrogen bonds N1—H1···N2 and additional weak hydrogen bonds C10—H10···O. S atoms of neighbouring molecules approach each other to 3.5267 (7) Å. Perpendicular to the ribbons are two C—H···π interactions (Table 1, Fig.2). The molecular structure of the title compound is depicted in Figure 1.

S2. Experimental

A mixture of butanoyl chloride (0.1 mol) and 2-aminobenzothiazole (0.1 mol) in anhydrous acetone (75 ml) was refluxed for 20 h. After cooling, the reaction mixture was poured in acidified cold water. The resulting dark brown solid was filtered and washed with cold acetone. Crystals of the title compound (I) suitable for X-Ray analysis were obtained after re-crystallization of the solid from ethanol (2.36 g, 79%). m.p.447 K.

S3. Refinement

The NH hydrogen was refined freely. Methyl H atoms were included on the basis of an idealized rigid group (C—H 0.98 Å, H—C—H 109.5°) allowed to rotate but not tip. Other hydrogen atoms were included using a riding model with C—H 0.95 (aromatic) or 0.99 (methylene) Å. U(H) values were fixed at 1.5U_{iso}(C) of the parent C atom for methyl H, 1.2U_{iso}(C) for other H.

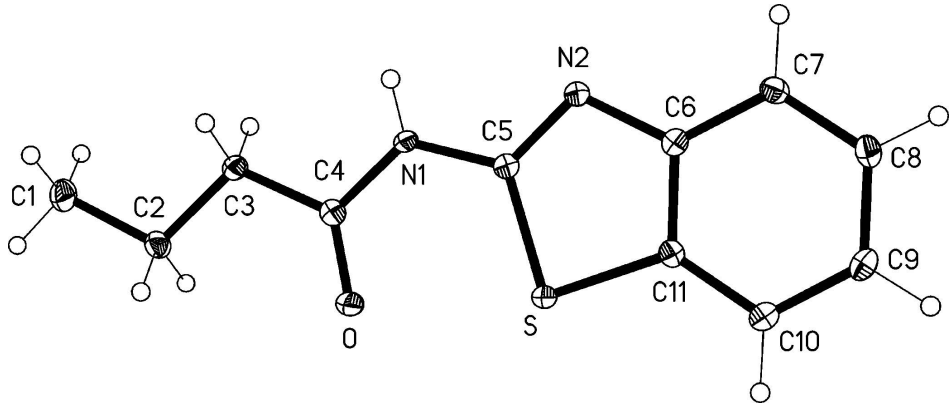

Figure 1

The molecular structure of the title compound. Ellipsoids represent 50% probability levels.

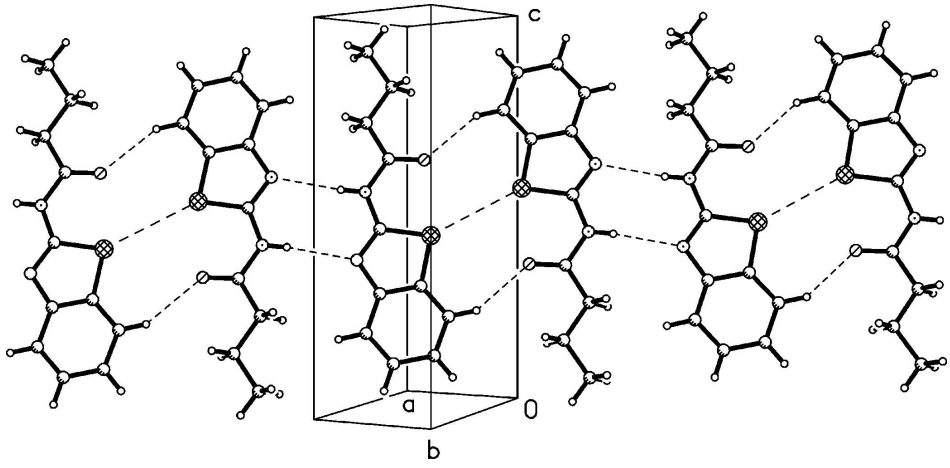

Figure 2

Packing diagram of I showing classical and "weak" H bonds and S···S contacts as thin dashed bonds. View direction is perpendicular to [$\bar{1}$02].

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Crystal data

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$M_r = 220.29$
Triclinic, $P\bar{1}$
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$a = 5.2916\ (4)$ Å
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$c = 13.565\ (1)$ Å
$\alpha = 92.618\ (7)°$
$\beta = 90.607\ (6)°$
$\gamma = 107.185\ (8)°$
$V = 509.92\ (8)$ Å^3
$Z = 2$
$F(000) = 232$
$D_x = 1.435$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4460 reflections
$\theta = 2.9–30.7°$
$\mu = 0.29$ mm^{-1}
$T = 100$ K
Plate, yellow
0.35 × 0.20 × 0.05 mm

Data collection

Oxford Diffraction Xcalibur S diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1057 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
T_{min} = 0.977, T_{max} = 1.000
8577 measured reflections
2728 independent reflections
2172 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 30.0°, θ_{min} = 2.9°
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 10$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 0.99
2728 reflections
141 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
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2]$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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.
Non-bonded distance
3.5267 (0.0007) S - S_$2 $2 - x + 2, -y + 1, -z + 1
Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)
- 2.9402 (0.0016) x + 6.9014 (0.0013) y + 2.6739 (0.0017) z = 1.5591 (0.0012)
* -0.0482 (0.0011) N1 * -0.0353 (0.0010) N2 * 0.0176 (0.0010) O * -0.0420 (0.0006) S * 0.0121 (0.0012) C1 * 0.0438 (0.0012) C2 * 0.0205 (0.0013) C3 * 0.0008 (0.0013) C4 * -0.0386 (0.0013) C5 * -0.0125 (0.0012) C6 * 0.0334 (0.0011) C7 * 0.0608 (0.0012) C8 * 0.0306 (0.0012) C9 * -0.0160 (0.0011) C10 * -0.0269 (0.0012) C11
Rms deviation of fitted atoms = 0.0332

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	0.3005 (2)	0.17657 (16)	0.43971 (8)	0.0115 (2)
H1	0.142 (3)	0.110 (2)	0.4321 (11)	0.019 (4)*
N2	0.2856 (2)	0.10743 (16)	0.60669 (8)	0.0110 (2)
O	0.65683 (18)	0.36649 (14)	0.36601 (7)	0.0168 (2)
S	0.74719 (6)	0.32370 (5)	0.55350 (2)	0.01216 (11)
C1	0.2219 (3)	0.2887 (2)	0.08646 (10)	0.0186 (3)
H1A	0.1669	0.1526	0.0710	0.028*
H1B	0.3186	0.3540	0.0309	0.028*
H1C	0.0653	0.3306	0.0981	0.028*

C2	0.4007 (3)	0.3337 (2)	0.17869 (9)	0.0141 (3)
H2A	0.5602	0.2931	0.1665	0.017*
H2B	0.4589	0.4715	0.1934	0.017*
C3	0.2581 (2)	0.2353 (2)	0.26720 (9)	0.0120 (3)
H3A	0.1017	0.2794	0.2799	0.014*
H3B	0.1935	0.0983	0.2506	0.014*
C4	0.4267 (2)	0.26838 (19)	0.35982 (9)	0.0118 (3)
C5	0.4162 (2)	0.19131 (19)	0.53257 (9)	0.0102 (3)
C6	0.4520 (2)	0.14896 (19)	0.69100 (9)	0.0109 (3)
C7	0.3830 (3)	0.0893 (2)	0.78621 (9)	0.0130 (3)
H7	0.2093	0.0123	0.7986	0.016*
C8	0.5711 (3)	0.1442 (2)	0.86165 (9)	0.0142 (3)
H8	0.5244	0.1051	0.9264	0.017*
C9	0.8288 (3)	0.2560 (2)	0.84506 (10)	0.0145 (3)
H9	0.9547	0.2907	0.8983	0.017*
C10	0.9017 (3)	0.3166 (2)	0.75156 (10)	0.0133 (3)
H10	1.0764	0.3922	0.7395	0.016*
C11	0.7103 (3)	0.26286 (19)	0.67562 (9)	0.0110 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0082 (5)	0.0137 (6)	0.0107 (5)	0.0002 (5)	−0.0016 (4)	0.0019 (4)
N2	0.0099 (5)	0.0118 (6)	0.0109 (5)	0.0026 (4)	0.0002 (4)	0.0006 (4)
O	0.0122 (4)	0.0210 (6)	0.0135 (5)	−0.0013 (4)	0.0001 (4)	0.0041 (4)
S	0.00957 (16)	0.0143 (2)	0.01083 (16)	0.00062 (12)	0.00010 (11)	0.00174 (12)
C1	0.0215 (7)	0.0210 (8)	0.0123 (6)	0.0046 (6)	−0.0013 (5)	0.0027 (6)
C2	0.0137 (6)	0.0167 (8)	0.0120 (6)	0.0043 (6)	0.0009 (5)	0.0029 (5)
C3	0.0106 (6)	0.0132 (7)	0.0118 (6)	0.0030 (5)	−0.0010 (5)	0.0010 (5)
C4	0.0130 (6)	0.0107 (7)	0.0122 (6)	0.0041 (5)	0.0009 (5)	0.0006 (5)
C5	0.0104 (6)	0.0090 (7)	0.0116 (6)	0.0034 (5)	0.0000 (4)	0.0006 (5)
C6	0.0115 (6)	0.0102 (7)	0.0120 (6)	0.0048 (5)	−0.0003 (5)	−0.0007 (5)
C7	0.0116 (6)	0.0137 (7)	0.0139 (6)	0.0036 (5)	0.0018 (5)	0.0025 (5)
C8	0.0164 (6)	0.0166 (8)	0.0110 (6)	0.0067 (6)	0.0008 (5)	0.0024 (5)
C9	0.0142 (6)	0.0155 (8)	0.0142 (6)	0.0055 (5)	−0.0040 (5)	−0.0007 (5)
C10	0.0123 (6)	0.0125 (7)	0.0148 (6)	0.0036 (5)	−0.0012 (5)	−0.0004 (5)
C11	0.0120 (6)	0.0111 (7)	0.0108 (6)	0.0048 (5)	0.0009 (4)	0.0013 (5)

Geometric parameters (Å, º)

N1—C4	1.3788 (16)	C9—C10	1.3858 (18)
N1—C5	1.3803 (16)	C10—C11	1.3956 (18)
N2—C5	1.3022 (16)	N1—H1	0.841 (17)
N2—C6	1.4015 (16)	C1—H1A	0.9800
O—C4	1.2209 (16)	C1—H1B	0.9800
S—C11	1.7351 (13)	C1—H1C	0.9800
S—C5	1.7501 (13)	C2—H2A	0.9900
C1—C2	1.5238 (18)	C2—H2B	0.9900

C2—C3	1.5236 (17)	C3—H3A	0.9900
C3—C4	1.5011 (17)	C3—H3B	0.9900
C6—C7	1.4019 (17)	C7—H7	0.9500
C6—C11	1.4027 (18)	C8—H8	0.9500
C7—C8	1.3802 (18)	C9—H9	0.9500
C8—C9	1.3988 (19)	C10—H10	0.9500

C4—N1—C5	123.92 (11)	C2—C1—H1B	109.5
C5—N2—C6	108.90 (10)	H1A—C1—H1B	109.5
C11—S—C5	87.62 (6)	C2—C1—H1C	109.5
C3—C2—C1	111.29 (11)	H1A—C1—H1C	109.5
C4—C3—C2	113.98 (11)	H1B—C1—H1C	109.5
O—C4—N1	121.46 (12)	C3—C2—H2A	109.4
O—C4—C3	124.23 (11)	C1—C2—H2A	109.4
N1—C4—C3	114.30 (11)	C3—C2—H2B	109.4
N2—C5—N1	121.66 (11)	C1—C2—H2B	109.4
N2—C5—S	118.00 (9)	H2A—C2—H2B	108.0
N1—C5—S	120.34 (9)	C4—C3—H3A	108.8
N2—C6—C7	126.34 (12)	C2—C3—H3A	108.8
N2—C6—C11	114.83 (11)	C4—C3—H3B	108.8
C7—C6—C11	118.83 (12)	C2—C3—H3B	108.8
C8—C7—C6	119.00 (12)	H3A—C3—H3B	107.7
C7—C8—C9	121.58 (12)	C8—C7—H7	120.5
C10—C9—C8	120.45 (12)	C6—C7—H7	120.5
C9—C10—C11	117.88 (12)	C7—C8—H8	119.2
C10—C11—C6	122.25 (12)	C9—C8—H8	119.2
C10—C11—S	127.12 (10)	C10—C9—H9	119.8
C6—C11—S	110.63 (9)	C8—C9—H9	119.8
C4—N1—H1	118.4 (11)	C9—C10—H10	121.1
C5—N1—H1	117.7 (11)	C11—C10—H10	121.1
C2—C1—H1A	109.5		

C1—C2—C3—C4	177.95 (12)	N2—C6—C7—C8	−179.52 (13)
C5—N1—C4—O	2.2 (2)	C11—C6—C7—C8	−0.1 (2)
C5—N1—C4—C3	−178.25 (12)	C6—C7—C8—C9	−0.6 (2)
C2—C3—C4—O	0.8 (2)	C7—C8—C9—C10	0.6 (2)
C2—C3—C4—N1	−178.73 (11)	C8—C9—C10—C11	0.2 (2)
C6—N2—C5—N1	−179.44 (12)	C9—C10—C11—C6	−1.0 (2)
C6—N2—C5—S	0.99 (15)	C9—C10—C11—S	178.35 (10)
C4—N1—C5—N2	177.35 (12)	N2—C6—C11—C10	−179.60 (12)
C4—N1—C5—S	−3.09 (18)	C7—C6—C11—C10	0.9 (2)
C11—S—C5—N2	−0.39 (11)	N2—C6—C11—S	0.99 (15)
C11—S—C5—N1	−179.97 (12)	C7—C6—C11—S	−178.49 (10)
C5—N2—C6—C7	178.19 (13)	C5—S—C11—C10	−179.73 (14)
C5—N2—C6—C11	−1.25 (17)	C5—S—C11—C6	−0.35 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.84 (2)	2.40 (2)	3.232 (2)	172 (1)
C10—H10···O^{ii}	0.95	2.46	3.277 (2)	144
C2—H2*B*···Cent(C6–C11)^{iii}	0.99	2.66	3.56	152
C3—H3*B*···Cent(C6–C11)^{iv}	0.99	2.64	3.47	142

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*, −*z*+1.