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3-[3-(3-Methoxybenzoyl)thioureido]propionic acid

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In the title compound, $C_{12}H_{14}N_2O_4S$, the dihedral angle between the 3-methoxybenzene and the central thiourea fragment is 7.18 (9)°. The molecule exhibits a *cis–trans* configuration with respect to the position of the propionic acid and methoxybenzoyl groups relative to the thiono S atom across the C—N bonds.

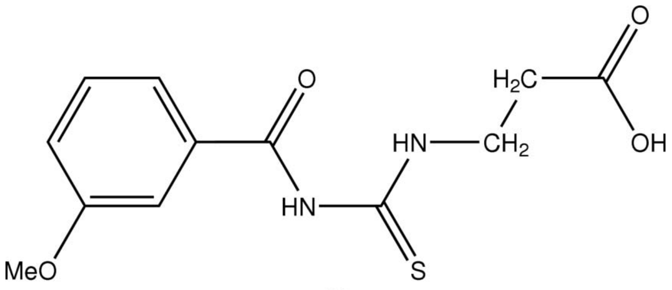
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.085
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, (I), is an isomer of 3-[3-(4-methoxybenzoyl)thioureido]propionic acid, (II) (Ngah *et al.*, 2006), with the methoxy group at the *meta* position of the benzoyl group. The molecules in (I) also have a *cis–trans* configuration with respect to the position of the propionic acid and methoxybenzoyl groups relative to the S1 atom across the C8—N2 and C8—N1 bonds, respectively (Fig. 1). The C11—C10—C9—N2 torsion angle of 63.4 (3)° is close to that observed in (II) [64.9 (4)°], indicating that the molecule mantains its *gauche* conformation about the C9—C10 bond. The bond lengths and angles are close to those observed in (II). The 4-methoxyphenyl [C1–C6/O1/C12 (*A*)] and carbonylthiourea [S1/O2/N1/N2/C7/C8 (*B*)] fragments are essentially planar. In the propionic acid fragment [O3/O4/C9/C10/C11 (*C*)], the maximum deviation from the mean plane is 0.151 (2) Å for atom C9. The dihedral angle between the least-squares planes of fragments *B*/*C* [66.34 (10)°] is close to that in (II) [65.34 (17)°] but the *A*/*C* dihedral angle of 61.15 (11)° is slightly larger [56.41 (18)° in (II)]. The *A*/*B* dihedral angle is 7.18 (9)°, smaller than the corresponding angle in (II) [10.78 (15)°].



(I)

There is an intramolecular hydrogen bond N2—H2···O2 (Table 1) which forms a pseudo-six membered ring (N2/H2/C8/N1/C7/O2). In the crystal structure, the molecules are linked by O—H···S, N—H···O and C—H···O intermolecular hydrogen bonds (Table 1), forming a one-dimensional chain along the *a* axis (Fig. 2).

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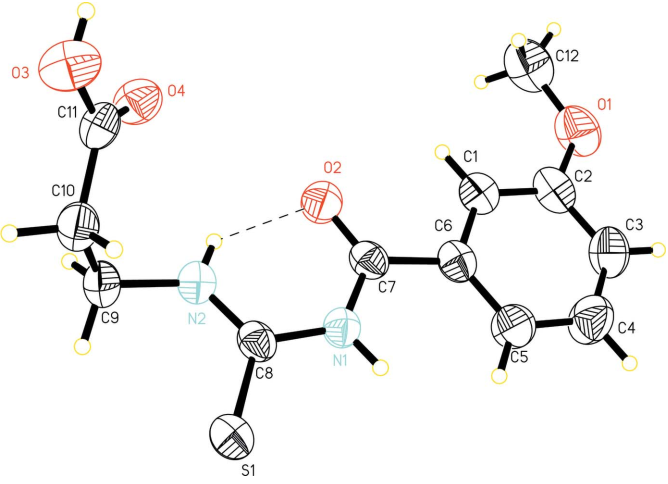

Figure 1
Molecular structure of (I), with displacement ellipsoids drawn at the 50% probablity level. The dashed line indicates the intramolecular hydrogen bond.

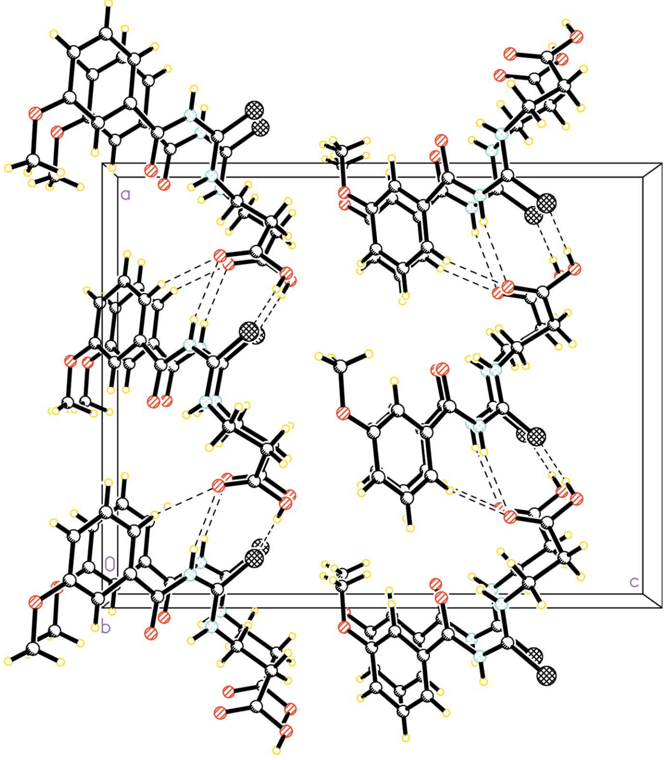

Figure 2
Molecular packing of (I) viewed down the *b* axis. Dashed lines indicate the intermolecular hydrogen bonds.

Experimental

A solution of 3-aminopropionic acid (0.05 mol, 4.45 g) in acetone was added dropwise to a two-necked round-bottomed flask containing an equimolar solution of 3-methoxybenzoyl isothiocyanate (0.05 mol, 9.65 g) in 20 ml of acetone. The mixture was refluxed for about 5 h. The light-yellow solution was filtered and some colourless crystals were obtained after five days of evaporation (yield 85%; m.p 430.3–431.1 K)

Crystal data

$C_{12}H_{14}N_2O_4S$
$M_r = 282.31$
Orthorhombic, $Pca2_1$
$a = 14.801$ (6) Å
$b = 4.8325$ (19) Å
$c = 18.624$ (8) Å
$V = 1332.1$ (9) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.26$ mm^{-1}
$T = 298$ (2) K
0.50 × 0.40 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.883$, $T_{\max} = 0.977$
6513 measured reflections
2297 independent reflections
2082 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.085$
$S = 1.09$
2297 reflections
174 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}
Absolute structure: Flack (1983), 958 Friedel pairs
Flack parameter: 0.02 (8)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$\cdots$O2	0.86	1.93	2.608 (3)	135
O3—H3$\cdots$S1$^{\rm i}$	0.82	2.30	3.116 (2)	177
N1—H1$\cdots$O4$^{\rm ii}$	0.86	2.26	3.109 (3)	167
C5—H5$\cdots$O4$^{\rm ii}$	0.93	2.29	3.188 (3)	161

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

H atoms on C were positioned geometrically with C—H 0.93, 0.96 and 0.97 Å, for aromatic, methlylene and methyl H atoms respectively, N—H = 0.86 Å, and O—H = 0.82 Å, and constrained to ride on their parent atoms with $U_{\rm iso}({\rm H}) = xU_{\rm eq}$(C,N,O), where $x = 1.5$ for methyl and hydroxyl H atoms and $x = 1.2$ for other H atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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