# organic compounds

# 3-Hydroxy-2-(4-methoxybenzene-sulfonamido)butanoic acid

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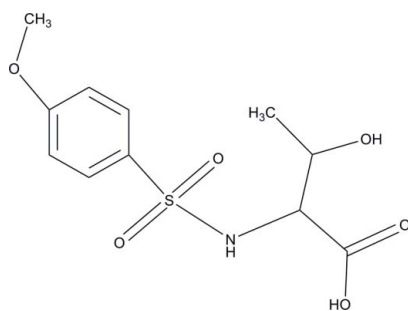
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The title compound, $C_{11}H_{15}NO_6S$, features a distorted tetrahedral geometry for the S atom. One of the sulfonamide O atoms is approximately coplanar with the benzene ring [C—C—S—O torsion angle = $-160.81\,(7)°$], whereas the other lies well below the plane [C—C—S—O = $-29.66\,(8)°$]. In the crystal, O—H···O and C—H···O hydrogen bonds link the molecules into chains parallel to the $b$ axis.

## Related literature

For details and applications of sulfonamides, see: Supuran *et al.* (2003); Scozzafava *et al.* (2003); Robinson *et al.* (2003); Delaet *et al.* (2003). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{11}H_{15}NO_6S$ | $b$ = 9.9204 (3) Å |
| $M_r$ = 289.30 | $c$ = 23.0561 (6) Å |
| Orthorhombic, $P2_12_12_1$ | $V$ = 1292.41 (7) Å$^3$ |
| $a$ = 5.6505 (2) Å | $Z$ = 4 |

Mo $K\alpha$ radiation
$\mu$ = 0.27 mm$^{-1}$
$T$ = 100 K
$0.75 \times 0.19 \times 0.17$ mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.821, $T_{max}$ = 0.954

35154 measured reflections
5756 independent reflections
5505 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
$S$ = 1.07
5756 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = $-0.42$ e Å$^{-3}$
Absolute structure: Flack (1983), 2444 Friedel pairs
Flack parameter: 0.02 (4)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H1$O5$···O6[i] | 0.844 (18) | 1.816 (19) | 2.6019 (10) | 154.3 (17) |
| O6—H1$O6$···O3[i] | 0.81 (2) | 1.99 (2) | 2.7990 (10) | 174.2 (19) |
| C5—H5$A$···O4[ii] | 0.93 | 2.52 | 3.3732 (11) | 153 |
| C8—H8$A$···O2[iii] | 0.98 | 2.48 | 3.4000 (11) | 156 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2664).

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**supplementary materials**

## 3-Hydroxy-2-(4-methoxybenzenesulfonamido)butanoic acid

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### Comment

The chemistry of sulfonamides is of interest as they show distinct physical, chemical and biological properties. Sulfonamides are used as anticancer, anti-inflammatory and antiviral agents (Supuran *et al.*, 2003; Scozzafava *et al.*, 2003). Amino acid-derived sulfonamides are shown to be active against Procollagen C-terminal protease, which is a member of the metzincin enzyme family (Robinson *et al.*, 2003; Delaet *et al.*, 2003).

The asymmetric unit of the title compound is shown in Fig. 1. The S atom is tetrahedrally bonded within a $CNO_2$ donor set with the greatest deviation manifested in the O2—S1—O3 angle of 120.08 (5)°. The sulfonamide O2 atom is approximately co-planar with the benzene ring [the O2-S1-C1-C6 torsion angle is -160.81 (7)°] whereas the O3 atom lies well below the plane [O3-S1-C1-C6 = -29.66 (8)°].

In the crystal structure (Fig. 2), intermolecular O—H···O and C—H···O hydrogen bonds (Table 1) link the molecules into chains parallel to the *b* axis.

### Experimental

To a solution of L-threonine (3 mmol, 0.618 g) in distilled water (10 ml), 4-methoxybenzene sulphonyl chloride (3 mmol, 0.357 g) was suspended. The pH of the solution was maintained at 8 by continuously adding 1M sodium carbonate solution throughout the reaction at room temperature. After the completion of the reaction, the pH was adjusted to 2 using 1N HCl solution which resulted in the formation of the precipitate which was filtered, dried and recrystallized in methanol to yield the title compound.

### Refinement

Atoms H1N1, H1O5 and H1O6 were located from a difference Fourier map and refined freely [N–H = 0.887 (17) and O–H = 0.81 (2)–0.845 (19) Å]. The remaining H atoms were positioned geometrically [C–H = 0.93–0.98 Å] and were refined using a riding model, with $U_{iso}(H) = 1.2$ or $1.5 U_{eq}(C)$. A rotating group model was applied to the methyl groups. 2444 Friedel pairs were used to determine the absolute configuration.
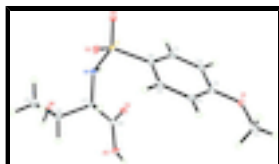
### Figures



Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids.
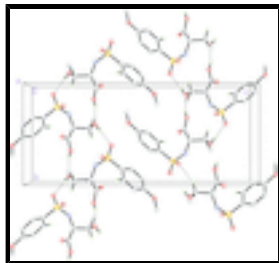
Fig. 2. The crystal packing of the title compound viewed along the *a* axis. H atoms not involved in hydrogen bonding (dashed lines) are omitted.

**3-Hydroxy-2-(4-methoxybenzenesulfonamido)butanoic acid**

*Crystal data*

| | |
|---|---|
| $C_{11}H_{15}NO_6S$ | $F(000) = 608$ |
| $M_r = 289.30$ | $D_x = 1.487$ Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 9845 reflections |
| $a = 5.6505$ (2) Å | $\theta = 3.4$–35.2° |
| $b = 9.9204$ (3) Å | $\mu = 0.27$ mm$^{-1}$ |
| $c = 23.0561$ (6) Å | $T = 100$ K |
| $V = 1292.41$ (7) Å$^3$ | Block, colourless |
| $Z = 4$ | $0.75 \times 0.19 \times 0.17$ mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 5756 independent reflections |
| Radiation source: fine-focus sealed tube | 5505 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.027$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 35.4°$, $\theta_{min} = 2.2°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $h = -7 \rightarrow 9$ |
| $T_{min} = 0.821$, $T_{max} = 0.954$ | $k = -16 \rightarrow 16$ |
| 35154 measured reflections | $l = -37 \rightarrow 37$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.073$ | $w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.163P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.07$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 5756 reflections | $\Delta\rho_{max} = 0.34$ e Å$^{-3}$ |
| 186 parameters | $\Delta\rho_{min} = -0.42$ e Å$^{-3}$ |

0 restraints

Primary atom site location: structure-invariant direct methods

Absolute structure: Flack (1983), 2444 Friedel pairs

Flack parameter: 0.02 (4)

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 ($Å^2$)*

|      | $x$          | $y$         | $z$          | $U_{iso}*/U_{eq}$ |
| ---- | ------------ | ----------- | ------------ | ----------------- |
| S1   | 0.72919 (4)  | 0.22850 (2) | 0.138337 (9) | 0.01332 (4)       |
| O1   | 0.78573 (15) | 0.61425 (7) | −0.05450 (3) | 0.02057 (13)      |
| O2   | 0.48689 (13) | 0.21583 (8) | 0.15597 (3)  | 0.01902 (13)      |
| O3   | 0.86556 (14) | 0.10991 (7) | 0.12458 (3)  | 0.01897 (13)      |
| O4   | 1.15328 (13) | 0.52453 (7) | 0.17150 (3)  | 0.02082 (14)      |
| O5   | 0.85821 (13) | 0.66432 (7) | 0.19810 (4)  | 0.01992 (14)      |
| O6   | 0.96165 (12) | 0.40568 (7) | 0.30315 (3)  | 0.01456 (11)      |
| N1   | 0.87145 (14) | 0.30287 (7) | 0.19112 (3)  | 0.01372 (12)      |
| C1   | 0.93213 (15) | 0.33833 (9) | 0.04102 (4)  | 0.01481 (14)      |
| H1A  | 1.0550       | 0.2771      | 0.0462       | 0.018*            |
| C2   | 0.94041 (16) | 0.43159 (9) | −0.00357 (4) | 0.01560 (14)      |
| H2A  | 1.0688       | 0.4326      | −0.0288      | 0.019*            |
| C3   | 0.75624 (17) | 0.52429 (8) | −0.01084 (3) | 0.01491 (14)      |
| C4   | 0.56040 (16) | 0.52178 (10)| 0.02592 (4)  | 0.01660 (15)      |
| H4A  | 0.4368       | 0.5824      | 0.0206       | 0.020*            |
| C5   | 0.55119 (15) | 0.42778 (9) | 0.07069 (4)  | 0.01495 (14)      |
| H5A  | 0.4214       | 0.4255      | 0.0955       | 0.018*            |
| C6   | 0.73634 (15) | 0.33731 (8) | 0.07829 (3)  | 0.01262 (12)      |
| C7   | 0.78523 (15) | 0.43593 (8) | 0.20919 (4)  | 0.01261 (13)      |
| H7A  | 0.6333       | 0.4522      | 0.1899       | 0.015*            |
| C8   | 0.74478 (15) | 0.44309 (8) | 0.27510 (3)  | 0.01324 (13)      |
| H8A  | 0.7047       | 0.5359      | 0.2858       | 0.016*            |
| C9   | 0.54836 (17) | 0.35081 (11)| 0.29434 (4)  | 0.02040 (17)      |
| H9A  | 0.5260       | 0.3595      | 0.3354       | 0.031*            |
| H9B  | 0.5891       | 0.2593      | 0.2852       | 0.031*            |
| H9C  | 0.4047       | 0.3748      | 0.2747       | 0.031*            |
| C10  | 0.95658 (16) | 0.54537 (9) | 0.19018 (4)  | 0.01371 (14)      |
| C11  | 0.6019 (2)   | 0.71196 (10)| −0.06293 (4) | 0.02317 (19)      |

| H11A | 0.6467 | 0.7728 | −0.0934 | 0.035* |
|------|--------|--------|---------|--------|
| H11B | 0.5782 | 0.7616 | −0.0277 | 0.035* |
| H11C | 0.4578 | 0.6668 | −0.0734 | 0.035* |
| H1N1 | 1.025 (3) | 0.3010 (15) | 0.1834 (7) | 0.025 (4)* |
| H1O5 | 0.952 (3) | 0.7296 (19) | 0.1933 (8) | 0.039 (5)* |
| H1O6 | 1.008 (4) | 0.462 (2) | 0.3261 (9) | 0.059 (6)* |

*Atomic displacement parameters ($Å^2$)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|----------|----------|----------|----------|----------|----------|
| S1 | 0.01979 (8) | 0.00881 (7) | 0.01137 (8) | −0.00184 (7) | −0.00180 (7) | 0.00073 (6) |
| O1 | 0.0300 (3) | 0.0169 (3) | 0.0149 (3) | 0.0028 (3) | 0.0028 (3) | 0.0051 (2) |
| O2 | 0.0214 (3) | 0.0182 (3) | 0.0175 (3) | −0.0080 (3) | 0.0000 (2) | 0.0032 (2) |
| O3 | 0.0322 (4) | 0.0089 (2) | 0.0157 (3) | 0.0027 (3) | −0.0047 (3) | −0.0007 (2) |
| O4 | 0.0202 (3) | 0.0154 (3) | 0.0269 (3) | 0.0005 (2) | 0.0100 (3) | 0.0002 (3) |
| O5 | 0.0183 (3) | 0.0094 (3) | 0.0321 (4) | 0.0004 (2) | 0.0039 (3) | 0.0003 (3) |
| O6 | 0.0156 (2) | 0.0127 (3) | 0.0154 (3) | −0.0003 (2) | −0.0030 (2) | −0.0036 (2) |
| N1 | 0.0178 (3) | 0.0104 (3) | 0.0130 (3) | 0.0009 (2) | −0.0027 (2) | −0.0016 (2) |
| C1 | 0.0166 (3) | 0.0127 (3) | 0.0151 (3) | 0.0023 (3) | 0.0001 (3) | −0.0012 (3) |
| C2 | 0.0184 (3) | 0.0147 (3) | 0.0137 (3) | 0.0010 (3) | 0.0032 (3) | −0.0002 (3) |
| C3 | 0.0209 (3) | 0.0123 (3) | 0.0115 (3) | 0.0005 (3) | 0.0006 (3) | 0.0010 (2) |
| C4 | 0.0181 (4) | 0.0163 (4) | 0.0153 (4) | 0.0037 (3) | 0.0000 (3) | 0.0035 (3) |
| C5 | 0.0151 (3) | 0.0158 (3) | 0.0139 (3) | 0.0013 (3) | 0.0007 (3) | 0.0014 (3) |
| C6 | 0.0159 (3) | 0.0107 (3) | 0.0113 (3) | 0.0000 (3) | −0.0006 (3) | 0.0007 (2) |
| C7 | 0.0147 (3) | 0.0097 (3) | 0.0135 (3) | 0.0002 (3) | −0.0003 (3) | −0.0006 (2) |
| C8 | 0.0129 (3) | 0.0135 (3) | 0.0133 (3) | 0.0009 (3) | 0.0010 (3) | −0.0013 (2) |
| C9 | 0.0155 (3) | 0.0252 (4) | 0.0206 (4) | −0.0034 (3) | 0.0036 (3) | 0.0027 (3) |
| C10 | 0.0163 (3) | 0.0113 (3) | 0.0136 (3) | 0.0005 (3) | 0.0007 (3) | 0.0002 (3) |
| C11 | 0.0355 (5) | 0.0165 (4) | 0.0175 (4) | 0.0033 (4) | −0.0036 (4) | 0.0037 (3) |

*Geometric parameters (Å, °)*

| S1—O2 | 1.4337 (8) | C2—H2A | 0.9300 |
|-------|-----------|--------|--------|
| S1—O3 | 1.4416 (7) | C3—C4 | 1.3940 (13) |
| S1—N1 | 1.6345 (8) | C4—C5 | 1.3922 (12) |
| S1—C6 | 1.7561 (8) | C4—H4A | 0.9300 |
| O1—C3 | 1.3555 (10) | C5—C6 | 1.3895 (12) |
| O1—C11 | 1.4338 (13) | C5—H5A | 0.9300 |
| O4—C10 | 1.2097 (11) | C7—C10 | 1.5193 (12) |
| O5—C10 | 1.3171 (11) | C7—C8 | 1.5385 (11) |
| O5—H1O5 | 0.845 (19) | C7—H7A | 0.9800 |
| O6—C8 | 1.4344 (11) | C8—C9 | 1.5055 (13) |
| O6—H1O6 | 0.81 (2) | C8—H8A | 0.9800 |
| N1—C7 | 1.4674 (11) | C9—H9A | 0.9600 |
| N1—H1N1 | 0.887 (17) | C9—H9B | 0.9600 |
| C1—C2 | 1.3839 (13) | C9—H9C | 0.9600 |
| C1—C6 | 1.4008 (12) | C11—H11A | 0.9600 |
| C1—H1A | 0.9300 | C11—H11B | 0.9600 |
| C2—C3 | 1.3989 (13) | C11—H11C | 0.9600 |

| | | | |
|---|---|---|---|
| O2—S1—O3 | 120.08 (5) | C1—C6—S1 | 120.41 (6) |
| O2—S1—N1 | 107.35 (4) | N1—C7—C10 | 110.45 (7) |
| O3—S1—N1 | 105.62 (4) | N1—C7—C8 | 111.80 (7) |
| O2—S1—C6 | 107.42 (4) | C10—C7—C8 | 110.28 (7) |
| O3—S1—C6 | 108.41 (4) | N1—C7—H7A | 108.1 |
| N1—S1—C6 | 107.35 (4) | C10—C7—H7A | 108.1 |
| C3—O1—C11 | 117.17 (8) | C8—C7—H7A | 108.1 |
| C10—O5—H1O5 | 113.7 (13) | O6—C8—C9 | 109.86 (7) |
| C8—O6—H1O6 | 113.2 (16) | O6—C8—C7 | 107.85 (7) |
| C7—N1—S1 | 117.01 (6) | C9—C8—C7 | 111.87 (7) |
| C7—N1—H1N1 | 113.6 (10) | O6—C8—H8A | 109.1 |
| S1—N1—H1N1 | 108.9 (10) | C9—C8—H8A | 109.1 |
| C2—C1—C6 | 119.16 (8) | C7—C8—H8A | 109.1 |
| C2—C1—H1A | 120.4 | C8—C9—H9A | 109.5 |
| C6—C1—H1A | 120.4 | C8—C9—H9B | 109.5 |
| C1—C2—C3 | 120.23 (8) | H9A—C9—H9B | 109.5 |
| C1—C2—H2A | 119.9 | C8—C9—H9C | 109.5 |
| C3—C2—H2A | 119.9 | H9A—C9—H9C | 109.5 |
| O1—C3—C4 | 124.11 (8) | H9B—C9—H9C | 109.5 |
| O1—C3—C2 | 115.49 (8) | O4—C10—O5 | 126.17 (9) |
| C4—C3—C2 | 120.39 (8) | O4—C10—C7 | 124.47 (8) |
| C5—C4—C3 | 119.50 (8) | O5—C10—C7 | 109.35 (7) |
| C5—C4—H4A | 120.2 | O1—C11—H11A | 109.5 |
| C3—C4—H4A | 120.2 | O1—C11—H11B | 109.5 |
| C6—C5—C4 | 119.87 (8) | H11A—C11—H11B | 109.5 |
| C6—C5—H5A | 120.1 | O1—C11—H11C | 109.5 |
| C4—C5—H5A | 120.1 | H11A—C11—H11C | 109.5 |
| C5—C6—C1 | 120.84 (8) | H11B—C11—H11C | 109.5 |
| C5—C6—S1 | 118.63 (6) | | |
| | | | |
| O2—S1—N1—C7 | −57.73 (7) | O3—S1—C6—C5 | 154.30 (7) |
| O3—S1—N1—C7 | 173.03 (6) | N1—S1—C6—C5 | −92.03 (7) |
| C6—S1—N1—C7 | 57.50 (7) | O2—S1—C6—C1 | −160.81 (7) |
| C6—C1—C2—C3 | 0.59 (13) | O3—S1—C6—C1 | −29.66 (8) |
| C11—O1—C3—C4 | −0.22 (13) | N1—S1—C6—C1 | 84.01 (8) |
| C11—O1—C3—C2 | −179.31 (8) | S1—N1—C7—C10 | −108.33 (7) |
| C1—C2—C3—O1 | 177.73 (8) | S1—N1—C7—C8 | 128.47 (6) |
| C1—C2—C3—C4 | −1.40 (14) | N1—C7—C8—O6 | 55.38 (9) |
| O1—C3—C4—C5 | −177.88 (9) | C10—C7—C8—O6 | −67.91 (8) |
| C2—C3—C4—C5 | 1.17 (14) | N1—C7—C8—C9 | −65.53 (9) |
| C3—C4—C5—C6 | −0.15 (14) | C10—C7—C8—C9 | 171.18 (7) |
| C4—C5—C6—C1 | −0.66 (13) | N1—C7—C10—O4 | −11.26 (12) |
| C4—C5—C6—S1 | 175.37 (7) | C8—C7—C10—O4 | 112.81 (10) |
| C2—C1—C6—C5 | 0.43 (13) | N1—C7—C10—O5 | 169.63 (7) |
| C2—C1—C6—S1 | −175.52 (7) | C8—C7—C10—O5 | −66.30 (9) |
| O2—S1—C6—C5 | 23.15 (8) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| O5—H1O5···O6[i] | 0.844 (18) | 1.816 (19) | 2.6019 (10) | 154.3 (17) |
| O6—H1O6···O3[i] | 0.81 (2) | 1.99 (2) | 2.7990 (10) | 174.2 (19) |
| C5—H5A···O4[ii] | 0.93 | 2.52 | 3.3732 (11) | 153. |
| C8—H8A···O2[iii] | 0.98 | 2.48 | 3.4000 (11) | 156. |

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

**Fig. 1**

**Fig. 2**