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1-(4-Methoxypyrimidin-2-yl)-3-(2-nitrophenylsulfonyl)urea

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.052
wR factor = 0.117
Data-to-parameter ratio = 13.4

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

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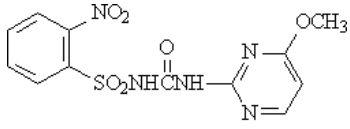
The title compound, $C_{12}H_{11}N_5O_6S$, has a basal plane, which contains a urea group and a pyrimidine ring. The S atom lies out of the plane of the urea moiety, and the S—N—C—N torsion angle is 160.6 (2)°. An extended π-conjugated system is formed between the urea moiety and the pyrimidine ring.

Comment

As successful herbicides, sulfonylureas have the advantages of low dosage, good crop selectivity and little mammalian toxicity. Since Levitt (1991) found the first one, tens of sulfonylureas have come on to the market. Levitt (1991) proposed the essential characteristics of these compounds, namely an aryl group, a bridge and a heterocycle. The highest level of activity was observed for sulfonylureas containing pyrimidin-2-yl or 1,3,5-triazin-2-yl groups which have two ower alkyl or alkoxy substituents (such as methyl or methoxy groups) on the 4- and 6-positions. We found, however, that phenylsulfonylureas, which have a pyrimidine ring containing only one substituent at the 4-position, show an almost equal level of activity (Li *et al.*, 1995). The crystal structures of some sulfonylureas have been determined to investigate the mechanism of action of sulfonylureas (Li *et al.*, 1992, 1993, 1994, 1997; Jiang *et al.*, 2000, 2002). We report here the structure of the title compound, (I).



(I)

Compound (I) has a basal plane involving the pyrimidine ring and the urea group, with a mean deviation of 0.02 Å (Fig. 1), but the S atom lies out of the plane of the urea moiety, with an S1—N1—C1—N2 torsion angle of 160.6 (2)°. In our earlier reports (Li *et al.*, 1993, 1994), the S atom, urea moiety and pyrimidine ring were coplanar. All N—C bonds (N1—C1, N2—C8 and N2—C1) in the urea bridge are shorter than a normal N—C length, but longer than a normal N=C bond (Table 1). The two N atoms (N1 and N2) are thus partially sp^2 hybridized, to form an extended π-conjugated system involving atom C1 and the pyrimidine ring. In addition, the intramolecular hydrogen bond N1—H···N3 results in a six-membered ring formed from atoms N3, C8, N2, C1, N1 and H (Table 2); this supports the coplanarity of the pyrimidine ring and the urea moiety.

Experimental

The title compound was synthesized by condensation of 2-nitrobenzenesulfonyl isocyanate and 2-amino-4-methoxypyrimidine (Li *et*

al., 1995). Single crystals of (I) suitable for crystallographic analysis were obtained from a DMF solution in an ether atmosphere.

Crystal data

$C_{12}H_{11}N_5O_6S$
M_r = 353.32
Triclinic, $P\overline{1}$
a = 5.470 (5) Å
b = 11.413 (7) Å
c = 12.131 (9) Å
α = 80.493 (6)°
β = 79.839 (8)°
γ = 76.896 (9)°
V = 719.8 (9) Å^3
Z = 2
D_x = 1.630 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 531 reflections
θ = 3.7–26.2°
μ = 0.27 mm^{-1}
T = 293 (2) K
Prism, colourless
0.32 × 0.24 × 0.20 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.796, T_{max} = 0.948
4129 measured reflections
2912 independent reflections
1846 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.7°
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 14$
$l = -15 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.117
S = 1.02
2912 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.1893P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.420 (2)	N3—C9	1.335 (3)
S1—N1	1.633 (3)	N5—O4	1.213 (3)
S1—C2	1.789 (3)	N5—O5	1.225 (3)
N1—C1	1.390 (4)	N5—C3	1.473 (4)
N2—C8	1.381 (3)	O1—C1	1.203 (3)
N2—C1	1.387 (4)	O6—C9	1.331 (3)
N3—C8	1.328 (4)	O6—C12	1.438 (3)
O2—S1—O3	119.19 (14)	C8—N2—C1	131.1 (2)
O2—S1—N1	109.24 (14)	O4—N5—C3	118.7 (3)
O2—S1—C2	106.56 (13)	C9—O6—C12	118.9 (2)
N1—S1—C2	105.40 (14)	O1—C1—N2	120.7 (3)
C1—N1—S1	122.61 (19)	N2—C1—N1	115.3 (2)
S1—N1—C1—N2	160.6 (2)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N3	0.86	2.02	2.653 (6)	130
N2—H2*A*···N4^{i}	0.86	2.05	2.904 (7)	178

Symmetry code: (i) $2-x, 2-y, -z$.

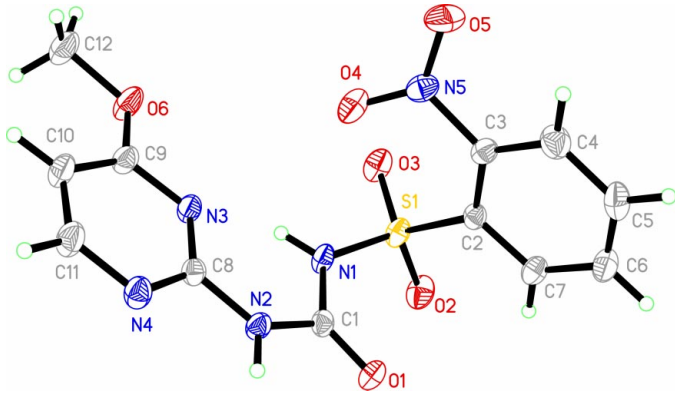


Figure 1
The molecular structure of (I), showing all non-H atoms with displacement ellipsoids drawn at the 30% probability level.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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