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2-(1*H*-Imidazol-1-yl)-3-isopropyl-1-benzothieno[3,2-*d*]pyrimidin-4(3*H*)-one

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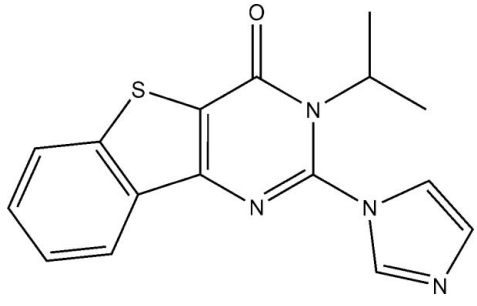
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.132; data-to-parameter ratio = 16.0.

In the title compound, $C_{16}H_{14}N_4OS$, the three fused rings of the benzothieno[3,2-*d*]pyrimidinone unit are essentially coplanar, the maximum deviation from the mean plane being 0.067 (3) Å. The dihedral angle between the mean plane of the fused rings and the imidazole ring is 72.00 (3)°. Offset π–π stacking interactions involving the fused rings are effective in the stabilization of the crystal structure. The centroid–centroid distances between the thienophene and benzene rings, and between the pyrimidine and benzene rings are 3.67 (1) and 3.93 (1) Å, respectively. There are two intramolecular C—H···O interactions.

Related literature

For related literature, see: Chambhare *et al.* (2003); Ding *et al.* (2004). For bond-length data, see: Allen *et al.* (1987). For related structures, see: Cao (2007); Xu *et al.* (2005, 2006).



Experimental

Crystal data

$C_{16}H_{14}N_4OS$
M_r = 310.37
Monoclinic, $P2_1/c$
a = 15.2759 (16) Å
b = 12.1387 (12) Å
c = 8.0172 (8) Å
β = 97.439 (2)°
V = 1474.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 (2) K
0.36 × 0.23 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
8864 measured reflections
3216 independent reflections
2657 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.08
3216 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16A···O1	0.96	2.38	2.963 (3)	119
C15—H15A···O1	0.96	2.45	3.046 (2)	120

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2265).

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supporting information

Acta Cryst. (2008). E**64**, o222 [https://doi.org/10.1107/S1600536807064598]

2-(1*H*-Imidazol-1-yl)-3-isopropyl-1-benzothieno[3,2-*d*]pyrimidin-4(3*H*)-one

Sheng-Zhen Xu

S1. Comment

Thienopyrimidine derivatives are of interest as possible antiviral agents, and because of their other biological properties, including antibacterial, antifungal, antiallergic and antiinflammatory activities (Chambhare *et al.*, 2003). We have recently focused on the synthesis of the fused heterocyclic systems containing thienopyrimidine *via* aza-Wittig reactions at room temperature (Ding *et al.*, 2004). We present here the structure of one such thienopyrimidine derivative, the title compound (I), (Fig. 1). Crystal structures of similar compounds have been reported (Cao, 2007; Xu *et al.*, 2005, 2006).

In the molecule of (I), the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). The three fused rings of (I) are essentially coplanar, the maximum deviation from the benzo[4,5]thieno[3,2-*e*]pyrimidinone mean plane being 0.067 (3) Å for atom N2. The dihedral angle between the three fused rings (S1/N1–2/C1–10) and imidazole ring B (N3–4/C11–13) is 72.00 (3)°.

Offset π-π stacking interactions, involving the rings; A (S1/C1/C6—C8), B (C1—C6) and C (N1—N2/C7—C10) are effective in the stabilization of the crystal structure. The adjacent thienophene ring A (S1/C1/C6—C8) and the benzene ring B (C1—C6) at (-*x*, 1 - *y*, 2 - *z*) have a centroid-centroid distance of 3.67 (1) Å The adjacent pyrimidine ring C (N2—N3/C10—C13) and the benzene ring B (C1—C6) at (-*x*, 1 - *y*, 2 - *z*) have a centroid-centroid distance of 3.93 (1) Å

S2. Experimental

The title compound was synthesized according to the literature method (Ding *et al.*, 2004). The product was recrystallized from ethanol/dichloromethane (1:2 *v*/*v*) at room temperature to give crystals suitable for single-crystal X-ray diffraction.

S3. Refinement

All H atoms were positioned geometrically, with C—H = 0.93–0.98 Å and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C), allowing for free rotation of the methyl groups.

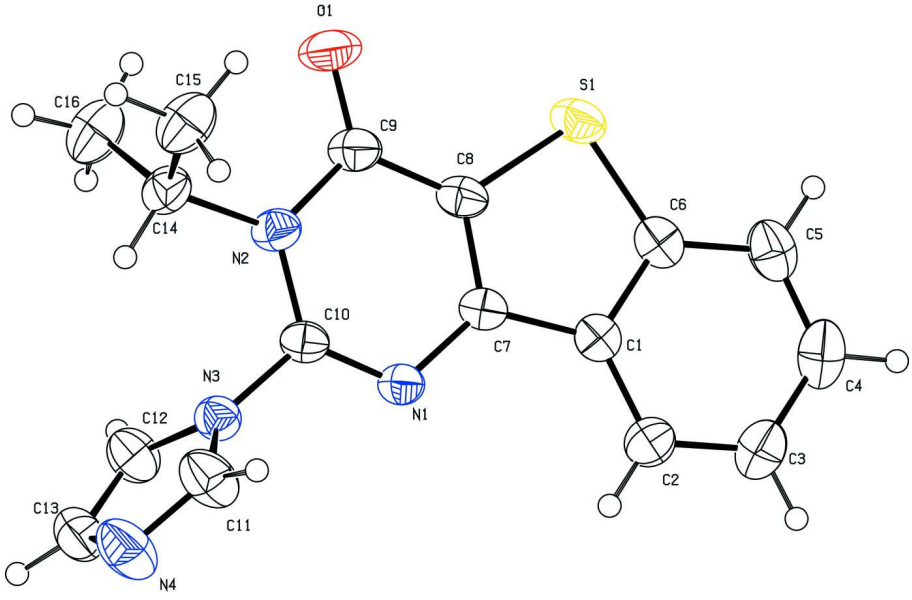

Figure 1

View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

2-(1*H*-Imidazol-1-yl)-3-isopropyl-1-benzothieno[3,2-*d*]pyrimidin-4(3*H*)-one

Crystal data

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$b = 12.1387\ (12)$ Å
$c = 8.0172\ (8)$ Å
$\beta = 97.439\ (2)°$
$V = 1474.1\ (3)$ Å^3
$Z = 4$
$F(000) = 648$
$D_x = 1.398$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3860 reflections
$\theta = 2.7–28.0°$
$\mu = 0.23$ mm^{-1}
$T = 298$ K
Block, colorless
0.36 × 0.23 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
8864 measured reflections
3216 independent reflections
2657 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.2°$
$h = -19\rightarrow16$
$k = -14\rightarrow15$
$l = -7\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.132$
$S = 1.08$
3216 reflections
201 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0813P)^2 + 0.01P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.017$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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.

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	0.01352 (10)	0.41878 (12)	0.82291 (18)	0.0377 (3)
C2	−0.04456 (11)	0.48730 (14)	0.7227 (2)	0.0477 (4)
H2	−0.0232	0.5438	0.6608	0.057*
C3	−0.13345 (12)	0.47032 (16)	0.7166 (3)	0.0591 (5)
H3	−0.1728	0.5158	0.6504	0.071*
C4	−0.16574 (12)	0.38522 (16)	0.8090 (3)	0.0641 (5)
H4	−0.2264	0.3750	0.8029	0.077*
C5	−0.10994 (12)	0.31650 (15)	0.9083 (3)	0.0567 (5)
H5	−0.1320	0.2601	0.9695	0.068*
C6	−0.01944 (11)	0.33330 (12)	0.9151 (2)	0.0435 (4)
C7	0.10839 (10)	0.41943 (11)	0.84835 (18)	0.0357 (3)
C8	0.14306 (10)	0.33777 (12)	0.95497 (19)	0.0404 (4)
C9	0.23580 (11)	0.32519 (13)	1.0012 (2)	0.0455 (4)
C10	0.24368 (10)	0.47907 (11)	0.81241 (18)	0.0368 (3)
C11	0.30832 (14)	0.65924 (14)	0.7549 (3)	0.0616 (5)
H11	0.2832	0.6983	0.8365	0.074*
C12	0.34470 (12)	0.52387 (15)	0.5998 (2)	0.0520 (4)
H12	0.3505	0.4548	0.5521	0.062*
C13	0.37967 (12)	0.61901 (15)	0.5549 (2)	0.0544 (4)
H13	0.4149	0.6261	0.4692	0.065*
C14	0.38228 (10)	0.41578 (14)	0.9892 (2)	0.0459 (4)
H14	0.4043	0.4766	0.9259	0.055*
C15	0.39582 (13)	0.44994 (16)	1.1717 (3)	0.0630 (5)
H15A	0.3672	0.3980	1.2370	0.095*
H15B	0.3710	0.5218	1.1827	0.095*
H15C	0.4579	0.4518	1.2114	0.095*
C16	0.43350 (13)	0.31491 (17)	0.9501 (3)	0.0676 (6)
H16A	0.4157	0.2533	1.0128	0.101*
H16B	0.4955	0.3281	0.9805	0.101*
H16C	0.4220	0.2991	0.8319	0.101*
N1	0.16018 (8)	0.48993 (10)	0.77008 (16)	0.0375 (3)
N2	0.28561 (8)	0.40583 (10)	0.92822 (16)	0.0402 (3)

N3	0.29862 (8)	0.54942 (10)	0.73057 (16)	0.0397 (3)
N4	0.35659 (12)	0.70387 (13)	0.6517 (2)	0.0699 (5)
O1	0.27164 (10)	0.25478 (10)	1.09671 (19)	0.0662 (4)
S1	0.06414 (3)	0.25652 (3)	1.02987 (6)	0.05010 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0434 (8)	0.0343 (7)	0.0358 (8)	−0.0020 (6)	0.0073 (6)	−0.0069 (6)
C2	0.0488 (9)	0.0438 (8)	0.0502 (10)	0.0038 (7)	0.0054 (7)	−0.0002 (7)
C3	0.0465 (10)	0.0589 (11)	0.0709 (13)	0.0070 (8)	0.0035 (9)	−0.0047 (9)
C4	0.0433 (10)	0.0640 (11)	0.0865 (15)	−0.0031 (9)	0.0140 (10)	−0.0157 (11)
C5	0.0538 (11)	0.0523 (10)	0.0672 (12)	−0.0111 (8)	0.0201 (9)	−0.0072 (9)
C6	0.0501 (9)	0.0383 (7)	0.0433 (9)	−0.0063 (7)	0.0112 (7)	−0.0071 (7)
C7	0.0438 (8)	0.0309 (7)	0.0317 (7)	−0.0031 (6)	0.0024 (6)	−0.0017 (6)
C8	0.0501 (9)	0.0343 (7)	0.0359 (8)	−0.0054 (6)	0.0022 (6)	0.0029 (6)
C9	0.0505 (9)	0.0401 (8)	0.0435 (9)	−0.0035 (7)	−0.0021 (7)	0.0067 (7)
C10	0.0447 (8)	0.0313 (7)	0.0337 (8)	−0.0021 (6)	0.0025 (6)	0.0000 (6)
C11	0.0814 (14)	0.0351 (8)	0.0741 (13)	−0.0054 (8)	0.0322 (11)	−0.0024 (8)
C12	0.0597 (11)	0.0528 (10)	0.0457 (10)	−0.0058 (8)	0.0147 (8)	−0.0054 (8)
C13	0.0521 (10)	0.0655 (11)	0.0472 (10)	−0.0090 (9)	0.0123 (8)	0.0030 (8)
C14	0.0402 (8)	0.0494 (9)	0.0459 (9)	0.0004 (7)	−0.0033 (7)	0.0003 (7)
C15	0.0559 (10)	0.0709 (12)	0.0573 (12)	0.0044 (9)	−0.0118 (9)	−0.0140 (9)
C16	0.0576 (11)	0.0676 (13)	0.0756 (14)	0.0157 (9)	0.0014 (10)	−0.0118 (10)
N1	0.0406 (7)	0.0349 (6)	0.0363 (7)	−0.0002 (5)	0.0029 (5)	0.0040 (5)
N2	0.0423 (7)	0.0381 (6)	0.0381 (7)	−0.0013 (5)	−0.0030 (5)	0.0029 (5)
N3	0.0409 (7)	0.0369 (6)	0.0411 (7)	−0.0022 (5)	0.0044 (5)	0.0016 (5)
N4	0.0847 (13)	0.0507 (9)	0.0801 (12)	−0.0141 (8)	0.0333 (10)	0.0046 (8)
O1	0.0630 (9)	0.0585 (8)	0.0717 (10)	−0.0013 (6)	−0.0118 (7)	0.0320 (6)
S1	0.0584 (3)	0.0417 (3)	0.0497 (3)	−0.01108 (17)	0.0051 (2)	0.01099 (17)

Geometric parameters (Å, º)

C1—C2	1.393 (2)	C10—N3	1.4166 (18)
C1—C6	1.405 (2)	C11—N4	1.296 (2)
C1—C7	1.437 (2)	C11—N3	1.353 (2)
C2—C3	1.368 (3)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.341 (2)
C3—C4	1.397 (3)	C12—N3	1.372 (2)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.371 (3)	C13—N4	1.363 (2)
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.392 (2)	C14—N2	1.499 (2)
C5—H5	0.9300	C14—C16	1.508 (2)
C6—S1	1.7437 (18)	C14—C15	1.509 (3)
C7—C8	1.370 (2)	C14—H14	0.9800
C7—N1	1.3713 (18)	C15—H15A	0.9600
C8—C9	1.425 (2)	C15—H15B	0.9600

C8—S1	1.7247 (15)	C15—H15C	0.9600
C9—O1	1.2279 (19)	C16—H16A	0.9600
C9—N2	1.4126 (19)	C16—H16B	0.9600
C10—N1	1.2835 (19)	C16—H16C	0.9600
C10—N2	1.3816 (18)		

C2—C1—C6	119.98 (14)	C13—C12—N3	105.79 (15)
C2—C1—C7	129.35 (14)	C13—C12—H12	127.1
C6—C1—C7	110.66 (13)	N3—C12—H12	127.1
C3—C2—C1	119.07 (16)	C12—C13—N4	110.89 (16)
C3—C2—H2	120.5	C12—C13—H13	124.6
C1—C2—H2	120.5	N4—C13—H13	124.6
C2—C3—C4	120.61 (18)	N2—C14—C16	112.49 (14)
C2—C3—H3	119.7	N2—C14—C15	110.11 (14)
C4—C3—H3	119.7	C16—C14—C15	114.53 (15)
C5—C4—C3	121.45 (17)	N2—C14—H14	106.4
C5—C4—H4	119.3	C16—C14—H14	106.4
C3—C4—H4	119.3	C15—C14—H14	106.4
C4—C5—C6	118.25 (17)	C14—C15—H15A	109.5
C4—C5—H5	120.9	C14—C15—H15B	109.5
C6—C5—H5	120.9	H15A—C15—H15B	109.5
C5—C6—C1	120.63 (16)	C14—C15—H15C	109.5
C5—C6—S1	126.75 (14)	H15A—C15—H15C	109.5
C1—C6—S1	112.62 (12)	H15B—C15—H15C	109.5
C8—C7—N1	122.53 (14)	C14—C16—H16A	109.5
C8—C7—C1	112.70 (13)	C14—C16—H16B	109.5
N1—C7—C1	124.70 (13)	H16A—C16—H16B	109.5
C7—C8—C9	122.07 (14)	C14—C16—H16C	109.5
C7—C8—S1	113.57 (12)	H16A—C16—H16C	109.5
C9—C8—S1	124.34 (11)	H16B—C16—H16C	109.5
O1—C9—N2	121.34 (15)	C10—N1—C7	115.30 (12)
O1—C9—C8	125.79 (15)	C10—N2—C9	119.78 (12)
N2—C9—C8	112.86 (12)	C10—N2—C14	121.25 (12)
N1—C10—N2	127.02 (13)	C9—N2—C14	118.78 (12)
N1—C10—N3	116.35 (12)	C11—N3—C12	106.00 (14)
N2—C10—N3	116.63 (12)	C11—N3—C10	125.99 (14)
N4—C11—N3	112.37 (17)	C12—N3—C10	127.67 (13)
N4—C11—H11	123.8	C11—N4—C13	104.96 (15)
N3—C11—H11	123.8	C8—S1—C6	90.44 (8)

C6—C1—C2—C3	0.4 (2)	C1—C7—N1—C10	178.52 (13)
C7—C1—C2—C3	179.29 (16)	N1—C10—N2—C9	6.4 (2)
C1—C2—C3—C4	−0.3 (3)	N3—C10—N2—C9	−173.15 (12)
C2—C3—C4—C5	0.1 (3)	N1—C10—N2—C14	−168.50 (14)
C3—C4—C5—C6	−0.1 (3)	N3—C10—N2—C14	11.9 (2)
C4—C5—C6—C1	0.2 (2)	O1—C9—N2—C10	175.54 (16)
C4—C5—C6—S1	−179.33 (14)	C8—C9—N2—C10	−5.9 (2)
C2—C1—C6—C5	−0.3 (2)	O1—C9—N2—C14	−9.4 (2)

C7—C1—C6—C5	−179.46 (14)	C8—C9—N2—C14	169.11 (13)
C2—C1—C6—S1	179.26 (12)	C16—C14—N2—C10	−119.77 (17)
C7—C1—C6—S1	0.14 (15)	C15—C14—N2—C10	111.16 (16)
C2—C1—C7—C8	−179.09 (15)	C16—C14—N2—C9	65.26 (19)
C6—C1—C7—C8	−0.07 (17)	C15—C14—N2—C9	−63.80 (18)
C2—C1—C7—N1	−1.9 (2)	N4—C11—N3—C12	−0.4 (2)
C6—C1—C7—N1	177.12 (13)	N4—C11—N3—C10	−174.04 (16)
N1—C7—C8—C9	4.5 (2)	C13—C12—N3—C11	0.6 (2)
C1—C7—C8—C9	−178.29 (13)	C13—C12—N3—C10	174.10 (15)
N1—C7—C8—S1	−177.29 (11)	N1—C10—N3—C11	70.9 (2)
C1—C7—C8—S1	−0.03 (17)	N2—C10—N3—C11	−109.48 (18)
C7—C8—C9—O1	179.45 (17)	N1—C10—N3—C12	−101.43 (18)
S1—C8—C9—O1	1.4 (3)	N2—C10—N3—C12	78.2 (2)
C7—C8—C9—N2	1.0 (2)	N3—C11—N4—C13	0.0 (2)
S1—C8—C9—N2	−177.07 (11)	C12—C13—N4—C11	0.4 (2)
N3—C12—C13—N4	−0.6 (2)	C7—C8—S1—C6	0.09 (12)
N2—C10—N1—C7	−0.9 (2)	C9—C8—S1—C6	178.31 (14)
N3—C10—N1—C7	178.70 (12)	C5—C6—S1—C8	179.44 (16)
C8—C7—N1—C10	−4.6 (2)	C1—C6—S1—C8	−0.14 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*A*···O1	0.96	2.38	2.963 (3)	119
C15—H15*A*···O1	0.96	2.45	3.046 (2)	120