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4-Methylsulfanyl-2-phenylquinazoline

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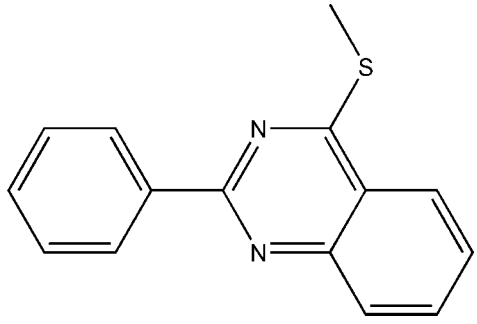
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.097; data-to-parameter ratio = 18.4.

In the title compound, $C_{15}H_{12}N_2S$, the methylthioquinazoline group is planar with the methyl C displaced by only 0.116 (3) Å from the plane of the quinazoline moiety. The dihedral angle between the phenyl ring and the quinazoline ring system is 13.95 (5)°. In the crystal, each molecule is linked by π–π stacking between to two adjacent inversion-related molecules. On one side, the inverted quinazoline groups interact with a centroid–centroid distance of 3.7105 (9) Å. On the other side, the quinazoline group interacts with the pyrimidine and phenyl rings of the second neighbour with centroid–centroid distances of 3.5287 (8) and 3.8601 (9) Å, respectively.

Related literature

For the synthesis of 4-alkythioqinazolines, see: Leonard & Curtin (1946); Hearn *et al.* (1951); Meerwein *et al.* (1956); Blatter & Lukaszewski (1964); Segarra *et al.* (1998); Smith *et al.* (2005*a*,*b*).



Experimental

Crystal data

$C_{15}H_{12}N_2S$
M_r = 252.33
Monoclinic, $P2_1/n$
a = 10.1951 (3) Å
b = 7.3545 (2) Å
c = 16.5300 (5) Å
β = 102.860 (3)°
V = 1208.33 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 150 K
0.23 × 0.18 × 0.15 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.848, T_{max} = 1.000
11140 measured reflections
3025 independent reflections
2558 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.08
3025 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5801).

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supporting information

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S1. Chemical context

S2. Structural commentary

In the 4-(methylthio)-2-phenylquinazoline molecule (Fig 1), the angle between the planes through the phenyl and phenyl-quinazoline ring systems is 13.95 (5)°. The molecules are stacked in the [010] direction with approximately parallel molecular planes. With no strong H-bond donors, one N atom accepts a long C—H···N contact linking molecules along [101]. The second N atom is not involved. 4-Methylthioquinazoline derivatives can be obtained from reaction of the potassium salt of 3*H*-quinazoline-4-thiones with iodomethane (Leonard & Curtin, 1946; Meerwein *et al.*, 1956). Quinazoline-4-thiones are produced from the corresponding 3*H*-quinazoline-4-ones using phosphorus pentasulfide (Hearn, *et al.*, 1951), Lawesson's reagent (Segarra *et al.*, 1998) or isothiocyanates (Blatter & Lukaszewski, 1964). In a continuation of our research focused on new synthetic routes towards novel substituted 4-alkylthioquinazoline derivatives (Smith *et al.*, 2005*a,b*) we have synthesized 4-(methylthio)-2-phenylquinazoline in a high yield (Smith *et al.*, 2005*a*).

S3. Supramolecular features

S4. Database survey

S5. Synthesis and crystallization

To a solution of 2-phenyl-3*H*-quinazoline-4-thione (4.81 g, 20.2 mmol) in a 1:1 mixture of MeOH and water (50 ml) containing KOH (3.0 g), was added iodomethane (3.41 g, 24.0 mmol). The reaction mixture was stirred for 20 min at room temperature and the solid obtained was filtered, washed with H_2O (3 × 30 ml), dried and recrystallized from Et_2O to give 4-(methylthio)-2-phenylquinazoline (4.63 g, 18.3 mmol, 91%) as colourless crystals, m.p. 93-94 °C [lit. 94 °C (H_2O); Meerwein *et al.*, 1956). ^{1}H NMR (400 MHz, $CDCl_3$, δ, p.p.m.) 8.70-8.66 (m, 2 H, ArH), 8.10-8.03 (m, 2 H, ArH), 7.83 (app. dt, J = 1, 8 Hz, 1 H, H-7), 7.58-7.51 (m, 4 H, ArH), 2.85 (s, 3 H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, d, p.p.m.) 171.8 (s, C-2), 159.2 (s, C-4), 149.1 (s, C-8a), 138.5 (s, C-1 of Ph), 133.9 (d, C-7), 131.0 (d, C-4 of Ph), 129.4 (d, C-8), 129.0 (d, C-3/C-5 of Ph), 128.9 (d, C-2/C-6 of Ph), 127.1 (d, C-6), 124.1 (d, C-5), 123.0 (s, C-4a), 13.0 (q, CH_3). EI—MS (*m/z*, %): 252 (M^+, 100), 251 (72), 205 (60), 102 (47), 77 (61), 51 (33). CI—MS (*m/z*, %): 253 (MH^+, 100), 207 (3). HRMS (CI): Calculated for $C_{15}H_{13}N_2S$ [*MH*] 253.0794; found, 253.0789.

S6. Refinement

H atoms were placed in calculated positions with C—H = 0.95 and 0.98 Å and refined in riding mode, U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for aromatic H atoms.

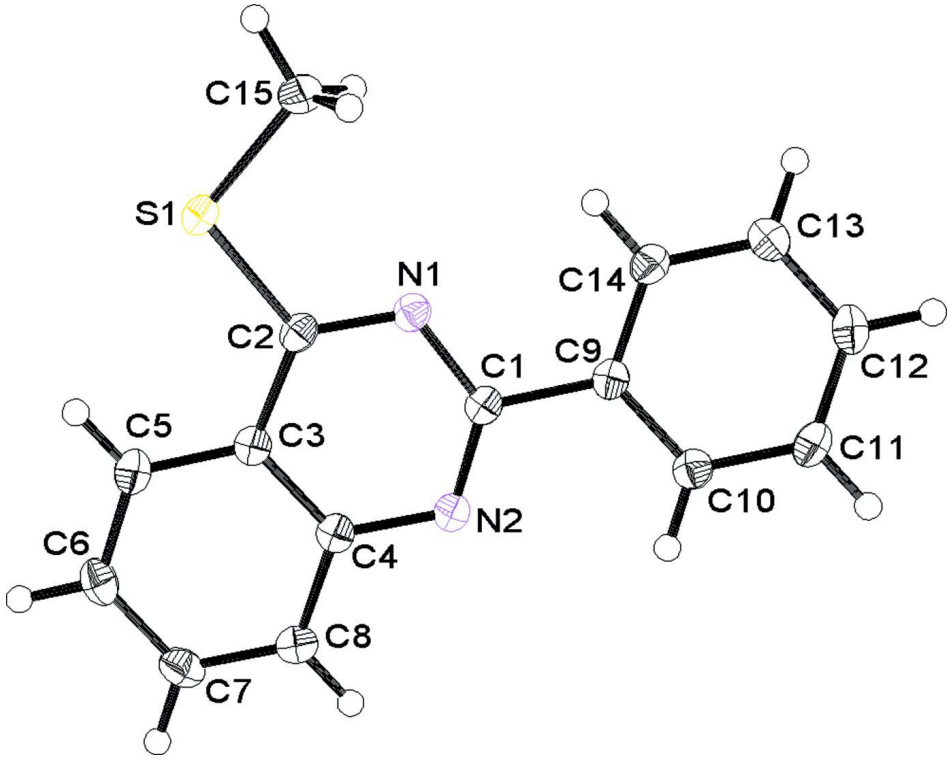

Figure 1

A molecule showing atom labels and 50% probability displacement ellipsoids for non-H atoms.

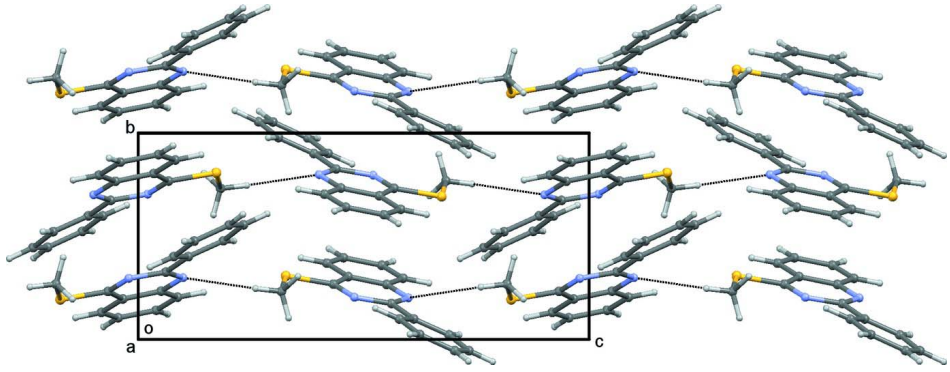

Figure 2

Packing diagram.

4-Methylsulfanyl-2-phenylquinazoline

Crystal data

$C_{15}H_{12}N_2S$
$M_r = 252.33$
Monoclinic, $P2_1/n$
$a = 10.1951$ (3) Å
$b = 7.3545$ (2) Å
$c = 16.5300$ (5) Å
$\beta = 102.860$ (3)°
$V = 1208.33$ (6) Å^3
$Z = 4$
$F(000) = 528$
$D_x = 1.387$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2558 reflections
$\theta = 3.1$–29.7°

μ = 0.25 mm^{-1}
T = 150 K

Block, colourless
0.23 × 0.18 × 0.15 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.848, T_{max} = 1.000

11140 measured reflections
3025 independent reflections
2558 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 29.7°, θ_{min} = 3.1°
h = −13→12
k = −9→10
l = −17→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.08
3025 reflections
164 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.6772P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.09137 (15)	0.6738 (2)	−0.06125 (9)	0.0182 (3)
C2	0.06916 (15)	0.7676 (2)	0.06700 (9)	0.0189 (3)
C3	−0.07074 (14)	0.8041 (2)	0.03446 (9)	0.0183 (3)
C4	−0.11800 (15)	0.7663 (2)	−0.05066 (9)	0.0196 (3)
C5	−0.16032 (16)	0.8695 (2)	0.08196 (10)	0.0229 (3)
H5	−0.1285	0.8950	0.1393	0.027*
C6	−0.29284 (16)	0.8957 (2)	0.04503 (10)	0.0257 (3)
H6	−0.3531	0.9391	0.0770	0.031*
C7	−0.34049 (16)	0.8591 (2)	−0.03973 (11)	0.0266 (4)
H7	−0.4328	0.8783	−0.0646	0.032*
C8	−0.25564 (15)	0.7960 (2)	−0.08710 (10)	0.0246 (3)
H8	−0.2892	0.7723	−0.1445	0.030*
C9	0.18424 (15)	0.5989 (2)	−0.11089 (9)	0.0188 (3)
C10	0.13360 (15)	0.5219 (2)	−0.18889 (9)	0.0213 (3)
H10	0.0394	0.5222	−0.2116	0.026*
C11	0.22001 (16)	0.4449 (2)	−0.23338 (9)	0.0237 (3)
H11	0.1846	0.3913	−0.2860	0.028*
C12	0.35767 (16)	0.4460 (2)	−0.20139 (10)	0.0253 (3)

H12	0.4166	0.3939	−0.2321	0.030*
C13	0.40914 (16)	0.5234 (2)	−0.12434 (10)	0.0250 (3)
H13	0.5036	0.5249	−0.1025	0.030*
C14	0.32309 (15)	0.5986 (2)	−0.07900 (9)	0.0225 (3)
H14	0.3589	0.6502	−0.0260	0.027*
C15	0.30675 (16)	0.7320 (3)	0.18247 (10)	0.0289 (4)
H15A	0.3070	0.6036	0.1666	0.043*
H15B	0.3564	0.7464	0.2401	0.043*
H15C	0.3498	0.8048	0.1460	0.043*
N1	0.14809 (12)	0.70406 (17)	0.02073 (8)	0.0191 (3)
N2	−0.03494 (12)	0.70111 (17)	−0.09896 (8)	0.0200 (3)
S1	0.13627 (4)	0.80726 (6)	0.17278 (2)	0.02388 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0219 (7)	0.0154 (7)	0.0174 (7)	−0.0014 (5)	0.0049 (6)	0.0015 (6)
C2	0.0237 (7)	0.0172 (7)	0.0156 (7)	−0.0014 (6)	0.0042 (6)	0.0017 (6)
C3	0.0216 (7)	0.0147 (7)	0.0191 (7)	−0.0010 (5)	0.0058 (6)	0.0020 (6)
C4	0.0218 (7)	0.0173 (7)	0.0202 (7)	−0.0011 (6)	0.0055 (6)	0.0014 (6)
C5	0.0282 (8)	0.0212 (8)	0.0208 (8)	0.0013 (6)	0.0088 (6)	0.0005 (6)
C6	0.0254 (8)	0.0229 (8)	0.0316 (9)	0.0035 (6)	0.0126 (7)	−0.0004 (7)
C7	0.0195 (7)	0.0261 (8)	0.0335 (9)	0.0018 (6)	0.0043 (6)	0.0005 (7)
C8	0.0222 (8)	0.0274 (9)	0.0231 (8)	−0.0008 (6)	0.0024 (6)	−0.0016 (7)
C9	0.0232 (7)	0.0161 (7)	0.0176 (7)	0.0008 (6)	0.0059 (6)	0.0026 (6)
C10	0.0229 (7)	0.0216 (8)	0.0195 (7)	−0.0004 (6)	0.0048 (6)	0.0022 (6)
C11	0.0318 (8)	0.0225 (8)	0.0174 (7)	−0.0004 (6)	0.0067 (6)	−0.0011 (6)
C12	0.0300 (8)	0.0234 (8)	0.0256 (8)	0.0037 (6)	0.0131 (7)	0.0006 (7)
C13	0.0226 (8)	0.0258 (9)	0.0274 (8)	0.0019 (6)	0.0071 (6)	0.0017 (7)
C14	0.0252 (8)	0.0230 (8)	0.0188 (7)	0.0001 (6)	0.0039 (6)	−0.0002 (6)
C15	0.0241 (8)	0.0406 (10)	0.0202 (8)	0.0037 (7)	0.0011 (6)	0.0014 (7)
N1	0.0209 (6)	0.0198 (6)	0.0171 (6)	−0.0007 (5)	0.0050 (5)	0.0019 (5)
N2	0.0218 (6)	0.0200 (6)	0.0185 (6)	−0.0005 (5)	0.0051 (5)	−0.0009 (5)
S1	0.0248 (2)	0.0308 (2)	0.0159 (2)	0.00122 (15)	0.00423 (15)	−0.00238 (16)

Geometric parameters (Å, º)

C1—N2	1.3153 (19)	C8—H8	0.9500
C1—N1	1.3680 (19)	C9—C14	1.396 (2)
C1—C9	1.4897 (19)	C9—C10	1.398 (2)
C2—N1	1.3134 (18)	C10—C11	1.388 (2)
C2—C3	1.433 (2)	C10—H10	0.9500
C2—S1	1.7544 (15)	C11—C12	1.385 (2)
C3—C4	1.410 (2)	C11—H11	0.9500
C3—C5	1.414 (2)	C12—C13	1.387 (2)
C4—N2	1.3730 (18)	C12—H12	0.9500
C4—C8	1.415 (2)	C13—C14	1.389 (2)
C5—C6	1.367 (2)	C13—H13	0.9500

C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.403 (2)	C15—S1	1.7970 (16)
C6—H6	0.9500	C15—H15A	0.9800
C7—C8	1.370 (2)	C15—H15B	0.9800
C7—H7	0.9500	C15—H15C	0.9800
N2—C1—N1	126.73 (13)	C10—C9—C1	120.56 (13)
N2—C1—C9	118.08 (13)	C11—C10—C9	120.43 (14)
N1—C1—C9	115.18 (13)	C11—C10—H10	119.8
N1—C2—C3	122.39 (13)	C9—C10—H10	119.8
N1—C2—S1	119.07 (11)	C12—C11—C10	120.27 (15)
C3—C2—S1	118.54 (11)	C12—C11—H11	119.9
C4—C3—C5	120.11 (14)	C10—C11—H11	119.9
C4—C3—C2	115.34 (13)	C11—C12—C13	119.80 (14)
C5—C3—C2	124.53 (14)	C11—C12—H12	120.1
N2—C4—C3	122.09 (13)	C13—C12—H12	120.1
N2—C4—C8	119.20 (14)	C12—C13—C14	120.23 (15)
C3—C4—C8	118.71 (13)	C12—C13—H13	119.9
C6—C5—C3	119.75 (15)	C14—C13—H13	119.9
C6—C5—H5	120.1	C13—C14—C9	120.38 (14)
C3—C5—H5	120.1	C13—C14—H14	119.8
C5—C6—C7	120.47 (14)	C9—C14—H14	119.8
C5—C6—H6	119.8	S1—C15—H15A	109.5
C7—C6—H6	119.8	S1—C15—H15B	109.5
C8—C7—C6	120.88 (15)	H15A—C15—H15B	109.5
C8—C7—H7	119.6	S1—C15—H15C	109.5
C6—C7—H7	119.6	H15A—C15—H15C	109.5
C7—C8—C4	120.08 (15)	H15B—C15—H15C	109.5
C7—C8—H8	120.0	C2—N1—C1	117.13 (13)
C4—C8—H8	120.0	C1—N2—C4	116.31 (13)
C14—C9—C10	118.88 (13)	C2—S1—C15	101.10 (7)
C14—C9—C1	120.52 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*B*···N2^{i}	0.98	2.67	3.648 (2)	173

Symmetry code: (i) $x+1/2, -y+3/2, z+1/2$.