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N-(3-Octyl-4-oxo-1,3-thiazolidin-2-ylidene)benzamide

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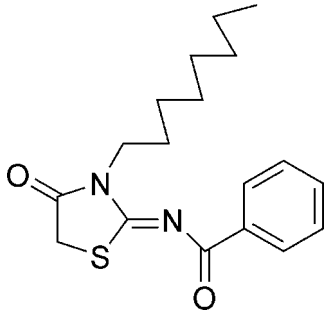
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.145; data-to-parameter ratio = 15.4.

In the title compound, $C_{18}H_{24}N_2O_2S$, the thiazolidinone ring is almost coplanar [maximum atomic deviation = 0.017 (3) Å], and is coplanar with the phenyl ring [dihedral angle = 0.62 (13)°]. The octyl group displays an extended conformation. In the crystal, weak intermolecular C—H···O hydrogen bonds link the molecules into supramolecular chains along [210].

Related literature

For pharmaceutical applications of thiazolidinones, see: Dwivedi *et al.* (1972); Chandrakant *et al.* (2004). For the synthesis, see: Peng *et al.* (2004).



Experimental

Crystal data

$C_{18}H_{24}N_2O_2S$
M_r = 332.45
Triclinic, $P\overline{1}$
a = 5.3342 (3) Å
b = 8.6196 (5) Å
c = 20.0775 (12) Å
α = 97.008 (5)°
β = 92.870 (4)°
γ = 99.477 (4)°
V = 901.41 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 293 K
0.26 × 0.18 × 0.16 mm

Data collection

Oxford Diffraction Nova A diffractometer
8685 measured reflections
3205 independent reflections
2371 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.145
S = 1.03
3205 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2^{i}	0.93	2.45	3.365 (4)	168

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5080).

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supporting information

Acta Cryst. (2010). E**66**, o3285 [https://doi.org/10.1107/S1600536810047884]

N-(3-Octyl-4-oxo-1,3-thiazolidin-2-ylidene)benzamide

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S1. Comment

Thiazolidinones have broad applications as anticonvulsant (Dwivedi *et al.*, 1972) and anti-microbial drugs (Chandrakant *et al.*, 2004). We report here the structure of a new thiazolidinone derivative, I, Fig. 2.

The thiazolidinyl ring and phenyl ring are almost co-planar with the dihedral angle of 0.67 (0.18)°. In the crystal structure, weak intermolecular C—H···O hydrogen bonds, Table 1, link the molecules to form one-dimensional supramolecular chains, Fig. 1.

S2. Experimental

The title compound was prepared followed to the procedure reported by Peng *et al.* (2004). NH_4SCN (0.152 g, 2 mmol) and [bmim][PF_4] (2 ml) was mixed in a 50 ml flask equipped with a dropping funnel and then was cooled in an ice-water bath. Next benzoyl chloride(0.284 g, 2 mmol) was added drop by drop and stirred for a further 20 min (disappearance of the raw material was monitored by TLC). n-Octylamine (2 mmol) was then added to the same reaction vessel at room temperature and the mixture was stirred for 20 min more. *N*-benzoyl-*N*′-octylthiourea was formed. After that, ethyl chloroacetate (2.4 mmol) and anhydrous sodium acetate (0.196 g, 2.4 mmol) was added to the flask, and the mixture was heated at 80°C for 2 h. The salts were firstly leached with water (10 ml×2), and the crude product was collected by filtration. Recrystallization from ethanol gave pure product as a yellow crystalline solid.

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.93-0.97 Å and refined in riding mode with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for the others.

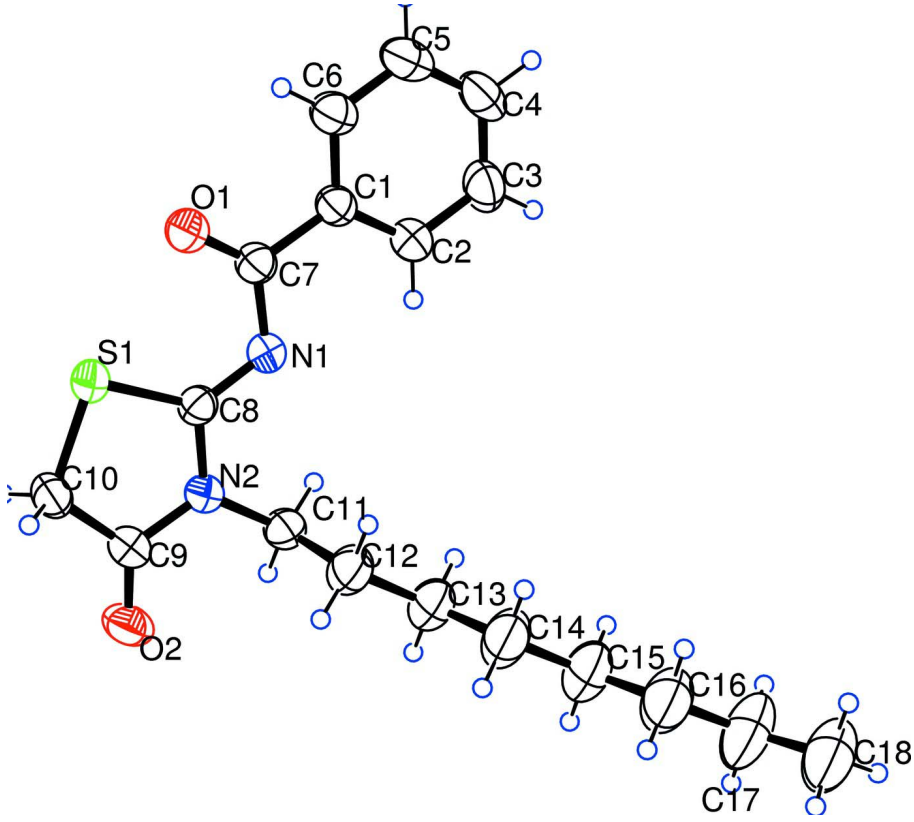

Figure 1

The molecular structure of the title compound with 40% probability displacement ellipsoids.

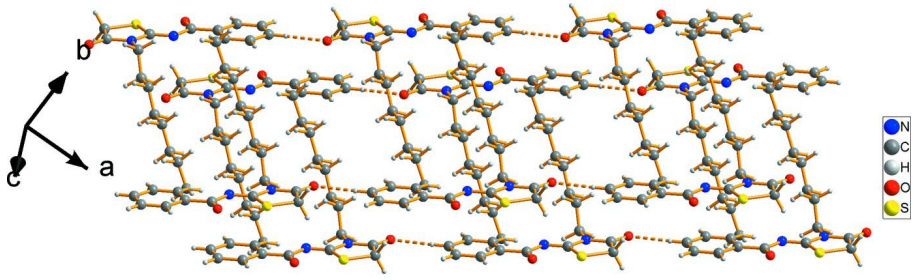

Figure 2

Crystal packing for I viewed down the *a* axis.

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Crystal data

$C_{18}H_{24}N_2O_2S$
$M_r = 332.45$
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$c = 20.0775\ (12)$ Å
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$\beta = 92.870\ (4)°$
$\gamma = 99.477\ (4)°$
$V = 901.41\ (9)$ Å^3
$Z = 2$
$F(000) = 356$
$D_x = 1.225$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2856 reflections
$\theta = 4.5–67.0°$
$\mu = 0.19$ mm^{-1}

T = 293 K
Prism, yellow

0.26 × 0.18 × 0.16 mm

Data collection

Oxford Diffraction Nova A diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
8685 measured reflections
3205 independent reflections

2371 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.1°, θ_{min} = 2.1°
h = −6→5
k = −9→10
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.145
S = 1.03
3205 reflections
208 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
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.4272P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
N2	0.2339 (4)	0.3596 (2)	0.30556 (10)	0.0496 (5)
N1	−0.1304 (4)	0.2176 (2)	0.34097 (10)	0.0492 (5)
C9	0.4393 (5)	0.4805 (3)	0.32305 (14)	0.0533 (6)
C8	0.0680 (5)	0.3283 (3)	0.35492 (12)	0.0464 (6)
C10	0.4427 (5)	0.5499 (3)	0.39502 (14)	0.0585 (7)
H10A	0.4422	0.6630	0.3982	0.070*
H10B	0.5952	0.5337	0.4197	0.070*
O1	−0.2580 (4)	0.2654 (2)	0.44909 (9)	0.0680 (6)
O2	0.5957 (4)	0.5200 (2)	0.28388 (11)	0.0733 (6)
S1	0.16338 (13)	0.45285 (8)	0.42998 (3)	0.0534 (2)
C7	−0.2882 (5)	0.1901 (3)	0.39283 (13)	0.0508 (6)
C1	−0.5089 (5)	0.0581 (3)	0.37455 (13)	0.0495 (6)
C11	0.1963 (5)	0.2715 (3)	0.23775 (13)	0.0569 (7)
H11A	0.1125	0.1638	0.2402	0.068*
H11B	0.3613	0.2663	0.2202	0.068*

C2	−0.5494 (5)	−0.0279 (3)	0.31152 (14)	0.0598 (7)
H2	−0.4341	−0.0064	0.2792	0.072*
C6	−0.6820 (5)	0.0229 (3)	0.42264 (15)	0.0606 (7)
H6	−0.6555	0.0795	0.4656	0.073*
C5	−0.8909 (6)	−0.0944 (4)	0.40707 (18)	0.0712 (8)
H5	−1.0049	−0.1172	0.4395	0.085*
C4	−0.9324 (6)	−0.1783 (4)	0.34373 (19)	0.0735 (9)
H4	−1.0759	−0.2565	0.3331	0.088*
C13	−0.0006 (7)	0.2535 (5)	0.12043 (15)	0.0816 (10)
H13A	0.1634	0.2576	0.1013	0.098*
H13B	−0.0658	0.1432	0.1241	0.098*
C12	0.0397 (6)	0.3448 (4)	0.18997 (14)	0.0730 (9)
H12A	0.1241	0.4523	0.1872	0.088*
H12B	−0.1249	0.3508	0.2077	0.088*
C3	−0.7605 (6)	−0.1462 (4)	0.29574 (17)	0.0721 (9)
H3	−0.7867	−0.2041	0.2530	0.086*
C15	−0.2276 (8)	0.2222 (6)	0.00389 (18)	0.1053 (13)
H15A	−0.2838	0.1109	0.0076	0.126*
H15B	−0.0679	0.2307	−0.0176	0.126*
C14	−0.1781 (8)	0.3108 (5)	0.07302 (17)	0.0976 (12)
H14A	−0.3401	0.3090	0.0930	0.117*
H14B	−0.1106	0.4207	0.0691	0.117*
C17	−0.4809 (10)	0.1911 (7)	−0.1089 (2)	0.1358 (19)
H17A	−0.5318	0.0792	−0.1055	0.163*
H17B	−0.3262	0.2022	−0.1326	0.163*
C16	−0.4209 (9)	0.2749 (6)	−0.04136 (19)	0.1114 (14)
H16A	−0.5784	0.2690	−0.0189	0.134*
H16B	−0.3621	0.3859	−0.0452	0.134*
C18	−0.6818 (9)	0.2415 (7)	−0.1504 (2)	0.1289 (18)
H18A	−0.7081	0.1765	−0.1933	0.193*
H18B	−0.6304	0.3505	−0.1567	0.193*
H18C	−0.8375	0.2302	−0.1280	0.193*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0480 (11)	0.0528 (12)	0.0450 (11)	0.0005 (10)	0.0052 (9)	0.0055 (9)
N1	0.0485 (11)	0.0499 (12)	0.0463 (12)	0.0009 (10)	0.0016 (9)	0.0058 (9)
C9	0.0484 (14)	0.0498 (15)	0.0606 (16)	0.0042 (12)	0.0051 (12)	0.0080 (12)
C8	0.0474 (13)	0.0485 (14)	0.0435 (13)	0.0085 (11)	0.0025 (10)	0.0074 (11)
C10	0.0509 (15)	0.0552 (16)	0.0643 (17)	−0.0023 (12)	−0.0024 (13)	0.0066 (13)
O1	0.0687 (12)	0.0731 (13)	0.0520 (11)	−0.0099 (10)	0.0110 (9)	−0.0052 (10)
O2	0.0613 (12)	0.0734 (14)	0.0804 (14)	−0.0074 (10)	0.0208 (11)	0.0104 (11)
S1	0.0525 (4)	0.0583 (4)	0.0445 (4)	0.0010 (3)	0.0008 (3)	−0.0002 (3)
C7	0.0477 (14)	0.0528 (15)	0.0519 (15)	0.0065 (12)	0.0025 (11)	0.0100 (12)
C1	0.0447 (13)	0.0500 (14)	0.0537 (15)	0.0063 (11)	0.0025 (11)	0.0099 (12)
C11	0.0572 (15)	0.0606 (16)	0.0497 (15)	0.0037 (13)	0.0105 (12)	0.0012 (13)
C2	0.0558 (16)	0.0597 (17)	0.0600 (17)	−0.0015 (13)	0.0014 (13)	0.0091 (14)

C6	0.0517 (15)	0.0645 (18)	0.0671 (18)	0.0083 (13)	0.0082 (13)	0.0153 (14)
C5	0.0541 (17)	0.073 (2)	0.089 (2)	0.0048 (15)	0.0147 (16)	0.0263 (18)
C4	0.0518 (16)	0.0626 (19)	0.102 (3)	−0.0080 (14)	−0.0050 (17)	0.0241 (18)
C13	0.088 (2)	0.097 (3)	0.0558 (18)	0.011 (2)	0.0007 (16)	0.0037 (17)
C12	0.077 (2)	0.086 (2)	0.0543 (17)	0.0132 (17)	0.0032 (15)	0.0036 (16)
C3	0.0703 (19)	0.0631 (19)	0.073 (2)	−0.0051 (15)	−0.0111 (16)	0.0013 (15)
C15	0.116 (3)	0.130 (4)	0.063 (2)	0.014 (3)	−0.010 (2)	0.004 (2)
C14	0.105 (3)	0.122 (3)	0.063 (2)	0.018 (2)	−0.0113 (19)	0.009 (2)
C17	0.153 (4)	0.185 (5)	0.068 (3)	0.049 (4)	−0.022 (3)	−0.004 (3)
C16	0.120 (3)	0.137 (4)	0.073 (2)	0.021 (3)	−0.012 (2)	0.006 (2)
C18	0.129 (4)	0.182 (5)	0.076 (3)	0.042 (4)	−0.017 (3)	0.003 (3)

Geometric parameters (Å, º)

N2—C9	1.380 (3)	C4—C3	1.384 (5)
N2—C8	1.383 (3)	C4—H4	0.9300
N2—C11	1.463 (3)	C13—C14	1.492 (5)
N1—C8	1.297 (3)	C13—C12	1.504 (4)
N1—C7	1.390 (3)	C13—H13A	0.9700
C9—O2	1.212 (3)	C13—H13B	0.9700
C9—C10	1.493 (4)	C12—H12A	0.9700
C8—S1	1.741 (2)	C12—H12B	0.9700
C10—S1	1.802 (3)	C3—H3	0.9300
C10—H10A	0.9700	C15—C14	1.489 (5)
C10—H10B	0.9700	C15—C16	1.502 (5)
O1—C7	1.221 (3)	C15—H15A	0.9700
C7—C1	1.493 (4)	C15—H15B	0.9700
C1—C2	1.374 (4)	C14—H14A	0.9700
C1—C6	1.395 (4)	C14—H14B	0.9700
C11—C12	1.503 (4)	C17—C16	1.451 (5)
C11—H11A	0.9700	C17—C18	1.477 (6)
C11—H11B	0.9700	C17—H17A	0.9700
C2—C3	1.384 (4)	C17—H17B	0.9700
C2—H2	0.9300	C16—H16A	0.9700
C6—C5	1.371 (4)	C16—H16B	0.9700
C6—H6	0.9300	C18—H18A	0.9600
C5—C4	1.373 (5)	C18—H18B	0.9600
C5—H5	0.9300	C18—H18C	0.9600
C9—N2—C8	116.6 (2)	C12—C13—H13A	108.5
C9—N2—C11	120.8 (2)	C14—C13—H13B	108.5
C8—N2—C11	122.6 (2)	C12—C13—H13B	108.5
C8—N1—C7	116.6 (2)	H13A—C13—H13B	107.5
O2—C9—N2	122.6 (3)	C11—C12—C13	113.0 (3)
O2—C9—C10	126.0 (2)	C11—C12—H12A	109.0
N2—C9—C10	111.4 (2)	C13—C12—H12A	109.0
N1—C8—N2	119.3 (2)	C11—C12—H12B	109.0
N1—C8—S1	128.94 (19)	C13—C12—H12B	109.0

N2—C8—S1	111.79 (18)	H12A—C12—H12B	107.8
C9—C10—S1	108.19 (18)	C2—C3—C4	119.8 (3)
C9—C10—H10A	110.1	C2—C3—H3	120.1
S1—C10—H10A	110.1	C4—C3—H3	120.1
C9—C10—H10B	110.1	C14—C15—C16	116.1 (4)
S1—C10—H10B	110.1	C14—C15—H15A	108.3
H10A—C10—H10B	108.4	C16—C15—H15A	108.3
C8—S1—C10	91.98 (12)	C14—C15—H15B	108.3
O1—C7—N1	125.0 (2)	C16—C15—H15B	108.3
O1—C7—C1	120.7 (2)	H15A—C15—H15B	107.4
N1—C7—C1	114.3 (2)	C15—C14—C13	117.1 (4)
C2—C1—C6	119.0 (2)	C15—C14—H14A	108.0
C2—C1—C7	122.1 (2)	C13—C14—H14A	108.0
C6—C1—C7	118.9 (2)	C15—C14—H14B	108.0
N2—C11—C12	113.0 (2)	C13—C14—H14B	108.0
N2—C11—H11A	109.0	H14A—C14—H14B	107.3
C12—C11—H11A	109.0	C16—C17—C18	116.8 (4)
N2—C11—H11B	109.0	C16—C17—H17A	108.1
C12—C11—H11B	109.0	C18—C17—H17A	108.1
H11A—C11—H11B	107.8	C16—C17—H17B	108.1
C1—C2—C3	120.5 (3)	C18—C17—H17B	108.1
C1—C2—H2	119.7	H17A—C17—H17B	107.3
C3—C2—H2	119.7	C17—C16—C15	118.6 (4)
C5—C6—C1	120.5 (3)	C17—C16—H16A	107.7
C5—C6—H6	119.7	C15—C16—H16A	107.7
C1—C6—H6	119.7	C17—C16—H16B	107.7
C6—C5—C4	120.2 (3)	C15—C16—H16B	107.7
C6—C5—H5	119.9	H16A—C16—H16B	107.1
C4—C5—H5	119.9	C17—C18—H18A	109.5
C5—C4—C3	119.9 (3)	C17—C18—H18B	109.5
C5—C4—H4	120.0	H18A—C18—H18B	109.5
C3—C4—H4	120.0	C17—C18—H18C	109.5
C14—C13—C12	115.2 (3)	H18A—C18—H18C	109.5
C14—C13—H13A	108.5	H18B—C18—H18C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.93	2.45	3.365 (4)	168

Symmetry code: (i) *x*−2, *y*−1, *z*.