Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(3-Bromopropyl)isoindoline-1,3-dione

Peng-Fei Cheng,[a] Chao-Jie Wang[a,b] and Yu-Xia Wang[a,b]*

[a]College of Chemistry and Chemical Engineering, Henan University, Kaifeng 475004, People's Republic of China, and [b]Key Laboratory of Natural Medicine and Immune Engineering, Henan University, Kaifeng 475004, People's Republic of China
Correspondence e-mail: hgxywyx@163.com

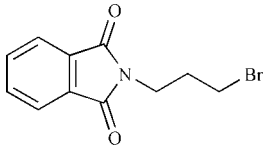
Received 18 September 2009; accepted 20 September 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.026; wR factor = 0.060; data-to-parameter ratio = 13.9.

In the title compound, $C_{11}H_{10}BrNO_2$, the dihedral angle between the five- and six-membered rings of the phthalamide system is 1.00 (16)°. There are no significant intermolecular interations except for van der Waals contacts.

Related literature

For pharmacological background on phthalamides, see: Brańa & Ramos (2001).



Experimental

Crystal data

$C_{11}H_{10}BrNO_2$ M_r = 268.11
Monoclinic, $P2_1$
a = 4.8413 (7) Å
b = 7.3401 (11) Å
c = 15.095 (2) Å
β = 91.729 (3)°
V = 536.18 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.81 mm^{-1}
T = 296 K
0.37 × 0.35 × 0.29 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.333, T_{max} = 0.405
2879 measured reflections
1888 independent reflections
1622 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.060
S = 1.00
1888 reflections
136 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 763 Friedel pairs
Flack parameter: 0.047 (11)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

This work was supported by the Basic Research Foundation for Natural Science of Henan University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5110).

References

Brańa, M. F. & Ramos, A. (2001). *Curr. Med. Chem. Anticancer Agents*, **1**, 237–255.
Bruker (2001). *SAINT-Plus*, *SMART* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2009). E**65**, o2646 [**doi:10.1107/S1600536809038021**]

2-(3-Bromopropyl)isoindoline-1,3-dione

P.-F. Cheng, C.-J. Wang and Y.-X. Wang

Comment

Phthalimides are well known cytotoxic DNA intercalating agents and have shown promise as potential anti-cancer agents (e.g. Brańa & Ramos, 2001). Its derivatives, such as bis-naphthalimides etc, represent a promising group of DNA-targeted anticancer agents, and the search for more potent analogues remains a priority. We now report the crystal structure of the title compound, (I).

As shown in Fig.1, the title compound consists of a phthalimide group supporting a bromopropane group. In the structure of (I), C11–O1 [1.210 (4) Å] and C4–O2 [1.208 (3) Å] are typical for a C==O double bond, the S(5) ring of N1/C4/C5/C10/C11 and the aromatic ring is approximatively coplanear, characterized by a dihedral angle of 1.00 (16)°.

Experimental

To a mixture of 1,3-dibromopropane (46 ml, 0.45 mol) and acetone (100 ml), potassium phthalimide (22.7 g, 0.15 mol) was added in batches with refluxing. After stirring for additional 12 h, the solid was filtered off, the solvent evaporated in vacuo. The residue was recrystallized in ethanol: evaporation gave (I) as colourless blocks (25.45 g, 63.4%).

Refinement

H atoms were placed geometrically with C—H = 0.93–0.97Å, and refined as riding with $U_{iso}(H)$=1.2U_{eq}(C).

Figures

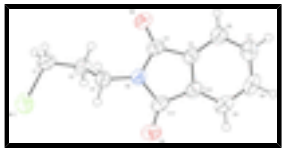


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

2-(3-Bromopropyl)isoindoline-1,3-dione

Crystal data

$C_{11}H_{10}BrNO_2$	F_{000} = 268
M_r = 268.11	D_x = 1.661 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 1480 reflections
a = 4.8413 (7) Å	θ = 2.8–24.1°
b = 7.3401 (11) Å	μ = 3.81 mm^{-1}

c = 15.095 (2) Å	T = 296 K
β = 91.729 (3)º	Block, colourless
V = 536.18 (14) Å^3	0.37 × 0.35 × 0.29 mm
Z = 2	

Data collection

Bruker SMART CCD diffractometer	1888 independent reflections
Radiation source: fine-focus sealed tube	1622 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
T = 296 K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.7º
Absorption correction: Multi-scan (SADABS; Bruker, 2001)	$h = -5 \rightarrow 4$
T_{min} = 0.333, T_{max} = 0.405	$k = -9 \rightarrow 8$
2879 measured reflections	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.026	$w = 1/[\sigma^2(F_o^2) + (0.0027P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.060	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
1888 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
136 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 763 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.047 (11)
Secondary atom site location: difference Fourier map	

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}
N1	0.6038 (5)	0.5266 (4)	0.75371 (15)	0.0421 (6)
Br1	0.85905 (7)	−0.00237 (6)	0.598616 (19)	0.06409 (14)
O1	0.9554 (5)	0.4693 (4)	0.85776 (14)	0.0650 (7)
O2	0.2346 (5)	0.6583 (3)	0.67773 (15)	0.0544 (6)
C1	0.6620 (7)	0.2145 (5)	0.5540 (2)	0.0525 (8)
H1A	0.7194	0.2405	0.4943	0.063*
H1B	0.4651	0.1897	0.5513	0.063*
C2	0.7160 (7)	0.3787 (4)	0.61137 (19)	0.0492 (8)
H2A	0.6288	0.4842	0.5838	0.059*
H2B	0.9134	0.4012	0.6154	0.059*
C3	0.6075 (7)	0.3556 (4)	0.7045 (2)	0.0489 (8)
H3A	0.4215	0.3064	0.7004	0.059*
H3B	0.7228	0.2685	0.7368	0.059*
C4	0.4095 (6)	0.6634 (4)	0.7365 (2)	0.0415 (7)
C5	0.4650 (6)	0.8063 (4)	0.80381 (19)	0.0398 (7)
C6	0.3321 (6)	0.9709 (5)	0.8172 (2)	0.0480 (8)
H6A	0.1856	1.0083	0.7803	0.058*
C7	0.4252 (8)	1.0770 (5)	0.8873 (2)	0.0567 (9)
H7A	0.3434	1.1896	0.8971	0.068*
C8	0.6392 (7)	1.0182 (7)	0.94342 (19)	0.0571 (9)
H8A	0.6951	1.0907	0.9912	0.068*
C9	0.7708 (7)	0.8541 (5)	0.9298 (2)	0.0514 (8)
H9A	0.9156	0.8158	0.9672	0.062*
C10	0.6813 (6)	0.7490 (4)	0.85924 (19)	0.0409 (7)
C11	0.7744 (7)	0.5670 (4)	0.82773 (19)	0.0464 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0494 (13)	0.0407 (19)	0.0357 (11)	0.0000 (12)	−0.0045 (10)	−0.0009 (12)
Br1	0.0801 (2)	0.0547 (2)	0.0575 (2)	0.0109 (2)	0.00154 (15)	−0.0067 (3)
O1	0.0724 (15)	0.0709 (18)	0.0506 (11)	0.0190 (15)	−0.0163 (11)	0.0038 (14)
O2	0.0581 (14)	0.0549 (14)	0.0491 (13)	0.0018 (11)	−0.0188 (11)	−0.0052 (11)
C1	0.061 (2)	0.054 (2)	0.0415 (17)	−0.0002 (15)	−0.0124 (16)	0.0022 (15)
C2	0.067 (2)	0.0421 (17)	0.0381 (16)	−0.0027 (15)	−0.0032 (15)	0.0027 (14)
C3	0.066 (2)	0.0390 (18)	0.0416 (16)	0.0025 (15)	−0.0022 (15)	0.0016 (14)
C4	0.0398 (17)	0.0461 (18)	0.0385 (16)	−0.0046 (14)	−0.0016 (14)	0.0050 (13)
C5	0.0417 (16)	0.0461 (17)	0.0316 (14)	−0.0081 (13)	0.0013 (12)	0.0027 (12)
C6	0.0529 (16)	0.048 (2)	0.0428 (14)	−0.0023 (16)	−0.0006 (12)	−0.0015 (17)
C7	0.069 (2)	0.0488 (18)	0.053 (2)	−0.0096 (16)	0.0114 (18)	−0.0059 (15)
C8	0.0614 (19)	0.069 (3)	0.0406 (15)	−0.019 (2)	0.0050 (14)	−0.015 (2)
C9	0.0483 (19)	0.069 (2)	0.0363 (16)	−0.0116 (17)	−0.0025 (15)	0.0002 (16)
C10	0.0424 (16)	0.0505 (17)	0.0300 (14)	−0.0065 (13)	0.0027 (13)	0.0042 (13)
C11	0.0519 (19)	0.0556 (19)	0.0314 (15)	−0.0024 (15)	−0.0024 (14)	0.0040 (13)

Geometric parameters (Å, °)

N1—C4	1.395 (4)	C3—H3B	0.9700
N1—C11	1.401 (4)	C4—C5	1.479 (4)
N1—C3	1.459 (4)	C5—C10	1.386 (4)
Br1—C1	1.965 (3)	C5—C6	1.387 (5)
O1—C11	1.210 (4)	C6—C7	1.379 (5)
O2—C4	1.208 (3)	C6—H6A	0.9300
C1—C2	1.503 (4)	C7—C8	1.387 (5)
C1—H1A	0.9700	C7—H7A	0.9300
C1—H1B	0.9700	C8—C9	1.381 (6)
C2—C3	1.525 (4)	C8—H8A	0.9300
C2—H2A	0.9700	C9—C10	1.374 (4)
C2—H2B	0.9700	C9—H9A	0.9300
C3—H3A	0.9700	C10—C11	1.492 (4)
C4—N1—C11	112.0 (3)	N1—C4—C5	106.0 (2)
C4—N1—C3	122.9 (2)	C10—C5—C6	121.5 (3)
C11—N1—C3	124.9 (3)	C10—C5—C4	108.5 (3)
C2—C1—Br1	112.2 (2)	C6—C5—C4	130.0 (3)
C2—C1—H1A	109.2	C7—C6—C5	117.5 (3)
Br1—C1—H1A	109.2	C7—C6—H6A	121.3
C2—C1—H1B	109.2	C5—C6—H6A	121.3
Br1—C1—H1B	109.2	C6—C7—C8	120.9 (4)
H1A—C1—H1B	107.9	C6—C7—H7A	119.5
C1—C2—C3	112.6 (3)	C8—C7—H7A	119.5
C1—C2—H2A	109.1	C9—C8—C7	121.3 (3)
C3—C2—H2A	109.1	C9—C8—H8A	119.3
C1—C2—H2B	109.1	C7—C8—H8A	119.3
C3—C2—H2B	109.1	C10—C9—C8	117.9 (3)
H2A—C2—H2B	107.8	C10—C9—H9A	121.0
N1—C3—C2	112.5 (3)	C8—C9—H9A	121.0
N1—C3—H3A	109.1	C9—C10—C5	120.8 (3)
C2—C3—H3A	109.1	C9—C10—C11	131.2 (3)
N1—C3—H3B	109.1	C5—C10—C11	108.0 (3)
C2—C3—H3B	109.1	O1—C11—N1	125.2 (3)
H3A—C3—H3B	107.8	O1—C11—C10	129.3 (3)
O2—C4—N1	124.6 (3)	N1—C11—C10	105.5 (3)
O2—C4—C5	129.4 (3)		
Br1—C1—C2—C3	−64.1 (4)	C7—C8—C9—C10	−0.8 (5)
C4—N1—C3—C2	74.3 (4)	C8—C9—C10—C5	−0.2 (5)
C11—N1—C3—C2	−111.8 (3)	C8—C9—C10—C11	−178.9 (3)
C1—C2—C3—N1	−167.3 (3)	C6—C5—C10—C9	0.2 (4)
C11—N1—C4—O2	−178.0 (3)	C4—C5—C10—C9	−178.1 (3)
C3—N1—C4—O2	−3.4 (5)	C6—C5—C10—C11	179.1 (3)
C11—N1—C4—C5	1.7 (3)	C4—C5—C10—C11	0.9 (3)
C3—N1—C4—C5	176.3 (3)	C4—N1—C11—O1	178.3 (3)
O2—C4—C5—C10	178.1 (3)	C3—N1—C11—O1	3.8 (5)
N1—C4—C5—C10	−1.6 (3)	C4—N1—C11—C10	−1.1 (3)

O2—C4—C5—C6	0.0 (5)	C3—N1—C11—C10	−175.6 (3)
N1—C4—C5—C6	−179.6 (3)	C9—C10—C11—O1	−0.5 (5)
C10—C5—C6—C7	0.7 (4)	C5—C10—C11—O1	−179.3 (3)
C4—C5—C6—C7	178.6 (3)	C9—C10—C11—N1	178.9 (3)
C5—C6—C7—C8	−1.7 (5)	C5—C10—C11—N1	0.1 (3)
C6—C7—C8—C9	1.7 (5)		

Fig. 1