Crystal structure of 3'-benzyloxy-2'-naphthyl-1-bromo-2-naphthoate, $C_{28}H_{19}BrO_3$

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Table 1. Data collection and handling.

Crystal:	pale yellow plate, size 0.1 × 0.95 × 1.05 mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	19.18 cm ⁻¹
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{\max}$:	55°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4866, 4593
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3037
$N(\text{param})_{\text{refined}}$:	289
Program:	SHELXTL [4]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(3)	4e	0.4967	1.0220	0.3019	0.08
H(4)	4e	0.4214	1.0839	0.4565	0.08
H(6)	4e	0.2694	1.1172	0.5317	0.08
H(7)	4e	0.1008	1.1034	0.5058	0.08
H(8)	4e	0.0009	1.0273	0.3124	0.08
H(9)	4e	0.0718	0.9618	0.1547	0.08
H(13)	4e	0.6814	0.9326	0.1624	0.08
H(15)	4e	0.8556	0.9187	0.1273	0.08
H(16)	4e	0.9619	0.8617	0.0120	0.08
H(17)	4e	0.8995	0.7697	-0.1664	0.08
H(18)	4e	0.7372	0.7307	-0.2145	0.08
H(20)	4e	0.5691	0.7373	-0.1633	0.08
H(22A)	4e	0.4562	0.6817	-0.0682	0.08
H(22B)	4e	0.3905	0.7234	-0.2208	0.08
H(24)	4e	0.2105	0.7534	-0.2425	0.08
H(25)	4e	0.0637	0.7160	-0.1860	0.08
H(26)	4e	0.0779	0.6322	0.0130	0.08
H(27)	4e	0.2329	0.5887	0.1558	0.08
H(28)	4e	0.3764	0.6279	0.1057	0.08

Abstract

$C_{28}H_{19}BrO_3$, monoclinic, $P12_1/c1$ (No. 14), $a = 13.769(1)$ Å, $b = 19.058(2)$ Å, $c = 8.716(1)$ Å, $\beta = 107.964(6)^\circ$, $V = 2175.7$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.059$, $wR_{\text{ref}}(F^2) = 0.164$, $T = 293$ K.

Source of material

The title compound was prepared according to [1] by esterification of the commercially available σ -1-bromonaphthoic acid [2] with the likewise known [3] 3-benzyloxy-2-naphthol. It is a useful intermediate in the synthesis of a twofold lactone bridged teraryl [1].

Discussion

Although the title compound is a useful synthetic precursor for the intramolecular biaryl coupling to link the bromine-bearing C-atom (C11) with C13 to give a six-membered lactone ring [1], it adopts a quite different conformation in the crystal, with C13 far away from the bromine (6.26 Å). The bromine is, in turn, quite close to the aromatic ring of the benzyl group, with ca. 4.50 Å distance as an average. Likewise remarkable is the non-coplanar array of the carboxyl unit (O1–C1–O12) with the naphthalene nucleus, with a significant dihedral angle between these two planes (58.1°), apparently due to the bulky bromine substituent at C11.

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Br	4e	0.18957(3)	0.89885(3)	-0.00974(5)	0.0636(3)	0.0927(4)	0.0755(3)	-0.0263(2)	0.0248(2)	-0.0305(2)
O(1)	4e	0.4020(2)	0.9405(1)	-0.0791(3)	0.059(2)	0.065(2)	0.049(1)	0.014(1)	0.019(1)	0.004(1)
C(1)	4e	0.4228(3)	0.9347(2)	0.0636(4)	0.045(2)	0.044(2)	0.048(2)	0.000(1)	0.015(1)	0.001(1)
C(2)	4e	0.3684(3)	0.9702(2)	0.1673(4)	0.045(2)	0.045(2)	0.045(2)	0.005(1)	0.015(1)	0.001(1)
C(3)	4e	0.4272(3)	1.0167(2)	0.2868(4)	0.041(2)	0.068(2)	0.059(2)	0.001(2)	0.014(2)	-0.014(2)
C(4)	4e	0.3820(3)	1.0534(2)	0.3787(4)	0.057(2)	0.072(2)	0.060(2)	-0.003(2)	0.013(2)	-0.019(2)
C(5)	4e	0.2778(3)	1.0471(2)	0.3610(4)	0.055(2)	0.062(2)	0.054(2)	0.010(2)	0.018(2)	-0.001(2)
C(6)	4e	0.2306(4)	1.0856(2)	0.4560(5)	0.071(3)	0.080(3)	0.069(2)	0.013(2)	0.029(2)	-0.013(2)
C(7)	4e	0.1299(4)	1.0780(3)	0.4401(6)	0.084(4)	0.101(3)	0.082(3)	0.023(3)	0.044(3)	-0.009(3)
C(8)	4e	0.0701(4)	1.0317(3)	0.3246(6)	0.058(3)	0.109(4)	0.092(3)	0.019(3)	0.041(2)	0.011(3)
C(9)	4e	0.1124(3)	0.9929(2)	0.2296(5)	0.053(2)	0.077(3)	0.073(2)	0.002(2)	0.026(2)	0.001(2)
C(10)	4e	0.2170(3)	0.9994(2)	0.2438(4)	0.046(2)	0.054(2)	0.049(2)	0.006(2)	0.016(2)	0.008(1)
C(11)	4e	0.2667(3)	0.9622(2)	0.1478(4)	0.047(2)	0.047(2)	0.047(2)	-0.003(2)	0.015(1)	-0.000(1)
O(12)	4e	0.5033(2)	0.8974(1)	0.1560(3)	0.050(1)	0.047(1)	0.047(1)	0.008(1)	0.016(1)	-0.0009(9)
C(12)	4e	0.5666(3)	0.8661(2)	0.0759(4)	0.048(2)	0.043(2)	0.044(2)	0.008(1)	0.015(1)	0.003(1)
C(13)	4e	0.6611(3)	0.8925(2)	0.1000(4)	0.050(2)	0.043(2)	0.049(2)	0.000(2)	0.012(1)	0.001(1)
C(14)	4e	0.7296(3)	0.8591(2)	0.0303(4)	0.041(2)	0.046(2)	0.053(2)	0.001(2)	0.011(1)	0.010(1)
C(15)	4e	0.8311(3)	0.8808(2)	0.0593(5)	0.051(2)	0.058(2)	0.069(2)	-0.004(2)	0.014(2)	0.005(2)
C(16)	4e	0.8944(3)	0.8473(2)	-0.0105(6)	0.046(2)	0.071(3)	0.093(3)	-0.002(2)	0.023(2)	0.007(2)
C(17)	4e	0.8572(3)	0.7914(2)	-0.1158(5)	0.054(2)	0.074(3)	0.092(3)	0.011(2)	0.036(2)	0.008(2)
C(18)	4e	0.7602(3)	0.7684(2)	-0.1450(5)	0.061(2)	0.060(2)	0.069(2)	0.001(2)	0.032(2)	-0.004(2)
C(19)	4e	0.6939(3)	0.8005(2)	-0.0722(4)	0.046(2)	0.046(2)	0.054(2)	0.002(2)	0.018(1)	0.004(1)
C(20)	4e	0.5931(3)	0.7752(2)	-0.0950(4)	0.047(2)	0.049(2)	0.059(2)	-0.002(2)	0.019(2)	-0.008(1)
C(21)	4e	0.5316(3)	0.8055(2)	-0.0187(4)	0.041(2)	0.048(2)	0.051(2)	-0.004(1)	0.015(1)	-0.002(1)
O(21)	4e	0.4366(2)	0.7825(1)	-0.0224(3)	0.045(1)	0.052(1)	0.070(1)	-0.007(1)	0.024(1)	-0.010(1)
C(22)	4e	0.4036(3)	0.7171(2)	-0.1058(5)	0.060(2)	0.055(2)	0.078(2)	-0.009(2)	0.030(2)	-0.016(2)
C(23)	4e	0.3081(3)	0.6944(2)	-0.0723(4)	0.048(2)	0.050(2)	0.057(2)	-0.006(2)	0.016(2)	-0.007(2)
C(24)	4e	0.2150(3)	0.7207(2)	-0.1613(5)	0.053(2)	0.081(3)	0.078(3)	0.004(2)	0.007(2)	-0.001(2)
C(25)	4e	0.1273(4)	0.6980(4)	-0.1286(8)	0.043(3)	0.138(5)	0.130(5)	-0.002(3)	0.007(3)	-0.050(4)
C(26)	4e	0.1363(5)	0.6480(4)	-0.0087(9)	0.093(5)	0.141(6)	0.141(6)	-0.066(4)	0.076(4)	-0.062(5)
C(27)	4e	0.2280(5)	0.6223(3)	0.0763(8)	0.125(6)	0.096(4)	0.105(4)	-0.043(4)	0.068(4)	-0.014(3)
C(28)	4e	0.3131(3)	0.6455(2)	0.0456(5)	0.071(3)	0.073(3)	0.064(2)	-0.004(2)	0.021(2)	0.000(2)

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