Crystal structures of *R*-(–)- and *S*-(+)-1-(4-amino-3,5-dichlorophenyl)-2-*tert*-butylaminoethanol hydrochloride, $(C_{12}H_{19}Cl_2N_2O)Cl$

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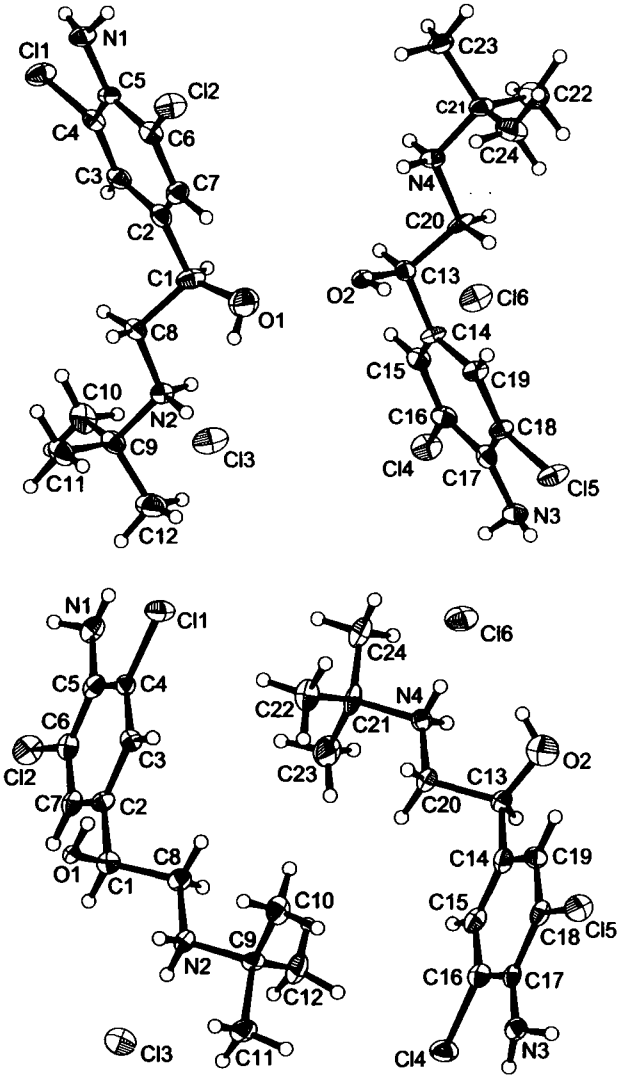

Abstract

$C_{12}H_{19}Cl_3N_2O$, triclinic, *P*1 (no. 1), $a = 6.894(3)$ Å, $b = 9.185(2)$ Å, $c = 12.070(4)$ Å, $\alpha = 76.01(2)°$, $\beta = 88.34(2)°$, $\gamma = 86.87(3)°$, $V = 740.4$ Å^3, $Z = 2$, $R_{gt}(F) = 0.058$, $wR_{ref}(F^2) = 0.170$, $T = 173$ K.

$C_{12}H_{19}Cl_3N_2O$, triclinic, *P*1 (no. 1), $a = 6.900(1)$ Å, $b = 9.195(2)$ Å, $c = 12.063(2)$ Å, $\alpha = 75.88(1)°$, $\beta = 88.47(2)°$, $\gamma = 86.89(2)°$, $V = 741.0$ Å^3, $Z = 2$, $R_{gt}(F) = 0.066$, $wR_{ref}(F^2) = 0.186$, $T = 173$ K.

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Source of materials

Synthesis according to [1] and separation using column chromatography with a chiral phase. Crystals of both the enantiomers were grown from a concentrated solution in an 1:1 methanol/toluene mixture, which was slowly evaporated at ambient temperature (m.p. 174-175 °C).

Discussion

Both enantiomers (known as *R*-(–)- and *S*-(+)-clenbuterol – figure, top and bottom, respectively) crystallize with two anion-cation pairs in the asymmetric unit. Their structural parameters are in good agreement, also with already published data of the racemic mixture [2]. Only the two dihedral O1–C1–C2–C7 angles are about 51° smaller than the corresponding O2–C13–C14–C15 angles. The Flack *x* parameters refined to values of each 0.0(1).

1. *R*-(–)-1-(4-amino-3,5-dichlorophenyl)-2-*tert*-butylaminoethanol hydrochloride, $(C_{12}H_{19}Cl_2N_2O)Cl$

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.3 × 0.4 × 0.6 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	6.09 cm^{-1}
Diffractometer, scan mode:	Siemens P4, $\omega/2\theta$
$2\theta_{max}$:	54.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6832, 6621
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 5121
$N(param)_{refined}$:	333
Programs:	SHELXS-97 [3], SHELXL-97 [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1)	1*a*	0.6512	0.4519	0.3619	0.030
H(1A)	1*a*	1.0139	0.4605	0.3659	0.050
H(3)	1*a*	0.4683	0.2902	0.2582	0.027
H(10)	1*a*	0.6267	–0.2690	0.4131	0.028
H(11)	1*a*	0.4870	–0.2171	0.3386	0.028
H(7)	1*a*	0.9736	0.1453	0.4186	0.026
H(8A)	1*a*	0.9052	0.4418	0.1718	0.024
H(8B)	1*a*	0.6785	0.4912	0.1658	0.024
H(20)	1*a*	0.9708	0.6511	0.2277	0.021
H(21)	1*a*	0.7632	0.6901	0.2474	0.021
H(10A)	1*a*	0.5696	0.6946	0.0424	0.035
H(10B)	1*a*	0.6236	0.8564	–0.0330	0.035
H(10C)	1*a*	0.5543	0.8371	0.0972	0.035
H(11A)	1*a*	1.0954	0.6660	0.0275	0.036
H(11B)	1*a*	0.9654	0.7588	–0.0761	0.036
H(11C)	1*a*	0.9064	0.5950	–0.0076	0.036
H(12A)	1*a*	0.8414	0.9492	0.1426	0.042

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(12B)	1*a*	0.9409	0.9697	0.0187	0.042
H(12C)	1*a*	1.0549	0.8771	0.1293	0.042
H(13)	1*a*	0.3476	0.6718	0.6302	0.023
H(2A)	1*a*	0.7164	0.5800	0.6240	0.019
H(15)	1*a*	0.2850	0.9347	0.5758	0.024
H(30)	1*a*	0.6491	1.3248	0.5776	0.025
H(31)	1*a*	0.7957	1.2772	0.6542	0.025
H(19)	1*a*	0.7941	0.7746	0.7343	0.022
H(20A)	1*a*	0.6041	0.5792	0.8195	0.026
H(20B)	1*a*	0.3791	0.6301	0.8284	0.026

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(40)	1*a*	0.5023	0.3828	0.7439	0.023
H(41)	1*a*	0.2965	0.4264	0.7636	0.023
H(22A)	1*a*	0.2804	0.3040	1.0635	0.036
H(22B)	1*a*	0.1741	0.4176	0.9586	0.036
H(22C)	1*a*	0.3669	0.4644	1.0092	0.036
H(23A)	1*a*	0.3933	0.1417	0.8266	0.029
H(23B)	1*a*	0.1927	0.1913	0.8801	0.029
H(23C)	1*a*	0.3527	0.0892	0.9613	0.029
H(24A)	1*a*	0.6807	0.3728	0.9612	0.041
H(24B)	1*a*	0.7082	0.2489	0.8882	0.041

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	1*a*	0.772(1)	0.4064(7)	0.3337(6)	0.018(3)	0.019(3)	0.036(4)	−0.003(2)	−0.005(3)	−0.001(3)
O(1)	1*a*	0.9187(6)	0.4224(5)	0.4053(3)	0.044(2)	0.038(2)	0.039(2)	−0.008(2)	−0.011(2)	−0.003(2)
C(2)	1*a*	0.728(1)	0.2441(6)	0.3365(5)	0.028(4)	0.017(3)	0.016(3)	0.002(2)	0.001(3)	−0.002(2)
C(3)	1*a*	0.558(1)	0.2111(7)	0.2926(6)	0.027(4)	0.017(3)	0.021(3)	0.000(3)	0.001(3)	0.001(2)
C(4)	1*a*	0.5169(9)	0.0648(7)	0.2982(5)	0.018(3)	0.021(3)	0.017(3)	0.000(3)	0.002(3)	−0.001(2)
Cl(1)	1*a*	0.2978(2)	0.0301(2)	0.2418(1)	0.0213(9)	0.0248(8)	0.039(1)	−0.0050(6)	−0.0082(7)	−0.0017(7)
C(5)	1*a*	0.638(1)	−0.0563(7)	0.3492(6)	0.020(3)	0.015(3)	0.021(3)	−0.005(2)	0.002(3)	−0.002(2)
N(1)	1*a*	0.6002(8)	−0.2072(5)	0.3534(5)	0.026(3)	0.011(2)	0.031(3)	−0.001(2)	−0.002(2)	−0.002(2)
C(6)	1*a*	0.8094(9)	−0.0236(6)	0.3928(5)	0.017(3)	0.015(3)	0.021(3)	0.006(2)	−0.001(3)	−0.001(2)
Cl(2)	1*a*	0.9714(2)	−0.1699(2)	0.4539(1)	0.0221(9)	0.0214(8)	0.042(1)	0.0047(6)	−0.0043(8)	−0.0021(7)
C(7)	1*a*	0.8556(9)	0.1256(7)	0.3875(6)	0.019(3)	0.023(3)	0.024(3)	−0.003(3)	−0.001(3)	−0.007(3)
C(8)	1*a*	0.7993(9)	0.4924(6)	0.2078(5)	0.022(3)	0.019(3)	0.017(3)	0.000(2)	0.002(2)	−0.002(2)
N(2)	1*a*	0.8477(7)	0.6516(5)	0.2001(4)	0.012(2)	0.016(2)	0.022(3)	0.002(2)	−0.003(2)	−0.002(2)
C(9)	1*a*	0.840(1)	0.7575(7)	0.0818(6)	0.025(4)	0.019(3)	0.021(3)	0.003(3)	0.003(3)	−0.001(3)
C(10)	1*a*	0.628(1)	0.7893(8)	0.0437(6)	0.025(4)	0.030(4)	0.028(4)	0.012(3)	−0.015(3)	0.001(3)
C(11)	1*a*	0.963(1)	0.6881(7)	−0.0010(6)	0.040(4)	0.027(4)	0.023(4)	0.002(3)	0.014(3)	−0.008(3)
C(12)	1*a*	0.927(1)	0.9011(7)	0.0942(7)	0.042(5)	0.023(3)	0.037(4)	−0.006(3)	0.005(3)	−0.001(3)
Cl(3)	1*a*	1.2795(2)	0.5767(2)	0.2576(2)	0.0177(9)	0.0282(9)	0.056(1)	0.0018(7)	−0.0046(8)	−0.0054(8)
C(13)	1*a*	0.482(1)	0.6689(6)	0.6608(5)	0.025(3)	0.014(3)	0.017(3)	0.000(2)	0.000(2)	−0.003(2)
O(2)	1*a*	0.6070(4)	0.5984(3)	0.5934(2)	0.018(1)	0.009(1)	0.021(1)	0.001(1)	−0.002(1)	−0.003(1)
C(14)	1*a*	0.5306(9)	0.8305(6)	0.6539(5)	0.013(3)	0.011(3)	0.029(3)	−0.003(2)	0.000(2)	−0.005(2)
C(15)	1*a*	0.4059(9)	0.9515(6)	0.6052(5)	0.021(3)	0.016(3)	0.021(3)	0.003(2)	−0.002(3)	−0.001(2)
C(16)	1*a*	0.4571(9)	1.0942(7)	0.5997(6)	0.022(4)	0.017(3)	0.025(4)	0.002(3)	0.001(3)	−0.001(3)
Cl(4)	1*a*	0.3014(2)	1.2474(1)	0.5391(1)	0.0288(9)	0.0155(7)	0.038(1)	0.0084(6)	−0.0064(8)	0.0001(6)
C(17)	1*a*	0.634(1)	1.1303(7)	0.6419(6)	0.027(4)	0.015(3)	0.016(3)	0.004(3)	0.003(3)	−0.006(2)
N(3)	1*a*	0.6801(8)	1.2742(5)	0.6410(5)	0.019(3)	0.016(2)	0.026(3)	0.000(2)	0.001(2)	−0.003(2)
C(18)	1*a*	0.7547(9)	1.0029(6)	0.6928(6)	0.014(3)	0.015(3)	0.026(4)	−0.001(2)	−0.004(3)	−0.004(2)
Cl(5)	1*a*	0.9743(2)	1.0361(2)	0.7477(1)	0.0219(9)	0.0206(8)	0.045(1)	−0.0057(6)	−0.0069(7)	−0.0053(7)
C(19)	1*a*	0.7083(9)	0.8562(6)	0.6996(5)	0.013(3)	0.014(3)	0.026(3)	0.003(2)	−0.003(2)	−0.002(2)
C(20)	1*a*	0.4752(9)	0.5808(6)	0.7850(6)	0.025(3)	0.005(2)	0.036(4)	−0.001(2)	−0.008(3)	−0.007(2)
N(4)	1*a*	0.4198(8)	0.4222(5)	0.7917(5)	0.019(3)	0.013(2)	0.025(3)	−0.001(2)	0.001(2)	−0.002(2)
C(21)	1*a*	0.4234(9)	0.3127(7)	0.9094(6)	0.020(3)	0.013(3)	0.023(3)	−0.002(2)	−0.005(3)	0.001(2)
C(22)	1*a*	0.300(1)	0.3807(7)	0.9926(6)	0.031(4)	0.021(3)	0.033(4)	0.006(3)	−0.003(3)	0.000(3)
C(23)	1*a*	0.332(1)	0.1710(6)	0.8929(6)	0.028(3)	0.016(3)	0.029(4)	−0.007(3)	−0.002(3)	−0.004(3)
C(24)	1*a*	0.630(1)	0.2814(8)	0.9475(7)	0.035(4)	0.029(4)	0.033(4)	−0.005(3)	0.000(3)	0.006(3)
Cl(6)	1*a*	0.9868(2)	0.4988(2)	0.7344(2)	0.0171(8)	0.0286(9)	0.046(1)	0.0033(7)	−0.0068(8)	−0.0081(8)

2. *S*-(+)-1-(4-amino-3,5-dichlorophenyl)-2-*tert*-butylamino-ethanol hydrochloride, $(C_{12}H_{19}Cl_2N_2O)Cl$

Table 4. Data collection and handling.

Crystal:	colorless block, size 0.4 × 0.5 × 0.7 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	6.09 cm^{-1}
Diffractometer, scan mode:	Siemens P4, $\omega/2\theta$
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6844, 6627
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 5705
$N(param)_{refined}$:	333
Programs:	SHELXS-97 [3], SHELXL-97 [4]

Table 5. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{iso}
H(1A)	1*a*	0.2747	0.1845	0.9098	0.022
H(1B)	1*a*	−0.0988	0.2648	0.9217	0.014
H(3)	1*a*	−0.1753	0.0794	0.8074	0.021
H(1C)	1*a*	−0.1679	−0.4239	0.8743	0.027
H(1D)	1*a*	−0.0394	−0.4806	0.9642	0.027
H(7)	1*a*	0.3355	−0.0790	0.9656	0.024
H(8A)	1*a*	0.0178	0.2766	0.7221	0.025

Table 5. Continued.

Atom	Site	x	y	z	U_{iso}
H(8B)	1a	0.2423	0.2253	0.7130	0.025
H(2A)	1a	0.3271	0.4294	0.7758	0.018
H(2B)	1a	0.1223	0.4729	0.7973	0.018
H(10A)	1a	−0.0214	0.6601	0.5264	0.033
H(10B)	1a	−0.0943	0.5996	0.6557	0.033
H(10C)	1a	−0.0636	0.4864	0.5741	0.033
H(11A)	1a	0.3008	0.7566	0.5750	0.030
H(11B)	1a	0.4172	0.6570	0.6825	0.030
H(11C)	1a	0.2059	0.7292	0.7004	0.030
H(12A)	1a	0.2570	0.3922	0.5318	0.038
H(12B)	1a	0.4468	0.4357	0.5874	0.038
H(12C)	1a	0.3476	0.5518	0.4807	0.038
H(1)	1a	−0.0314	0.4080	0.1771	0.030
H(2C)	1a	−0.3669	0.3665	0.1731	0.060
H(15)	1a	0.1481	0.5649	0.2849	0.029
H(3A)	1a	−0.0115	1.1258	0.1287	0.025

Table 5. Continued.

Atom	Site	x	y	z	U_{iso}
H(3B)	1a	0.1378	1.0806	0.1966	0.025
H(19)	1a	−0.3546	0.7146	0.1234	0.025
H(20A)	1a	−0.0538	0.3662	0.3754	0.024
H(20B)	1a	−0.2806	0.4156	0.3714	0.024
H(4A)	1a	−0.1401	0.1674	0.2940	0.024
H(4B)	1a	−0.3476	0.2070	0.3122	0.024
H(22A)	1a	−0.2811	0.2583	0.5508	0.033
H(22B)	1a	−0.3433	0.0944	0.6175	0.033
H(22C)	1a	−0.4728	0.1916	0.5149	0.033
H(23A)	1a	0.0605	0.0128	0.4493	0.043
H(23B)	1a	−0.0109	0.0075	0.5775	0.043
H(23C)	1a	0.0477	0.1632	0.4942	0.043
H(24A)	1a	−0.4446	−0.0225	0.4248	0.039
H(24B)	1a	−0.2977	−0.1202	0.5177	0.039
H(24C)	1a	−0.2375	−0.0804	0.3850	0.039

Table 6. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	1a	0.1410(8)	0.1877(6)	0.8791(5)	0.013(2)	0.020(2)	0.022(3)	0.003(2)	0.005(2)	−0.008(2)
O(1)	1a	0.0139(4)	0.2558(3)	0.9480(2)	0.011(1)	0.012(1)	0.012(1)	0.0008(9)	0.0019(8)	−0.0030(9)
C(2)	1a	0.0901(7)	0.0258(5)	0.8866(5)	0.012(2)	0.019(3)	0.022(3)	0.000(2)	0.004(2)	−0.005(2)
C(3)	1a	−0.0886(7)	−0.0018(6)	0.8419(5)	0.012(2)	0.023(3)	0.018(3)	0.003(2)	0.000(2)	−0.007(2)
C(4)	1a	−0.1350(7)	−0.1473(6)	0.8492(4)	0.015(2)	0.021(2)	0.014(3)	−0.000(2)	0.000(2)	−0.004(2)
Cl(1)	1a	−0.3534(2)	−0.1799(2)	0.7940(1)	0.0211(7)	0.0256(7)	0.0387(8)	−0.0058(5)	−0.0033(6)	−0.0055(6)
C(5)	1a	−0.0096(7)	−0.2728(4)	0.8997(4)	0.029(3)	0.015(2)	0.020(3)	−0.003(2)	0.009(2)	−0.007(2)
N(1)	1a	−0.0577(6)	−0.4197(4)	0.9008(4)	0.027(2)	0.013(2)	0.025(2)	0.003(2)	0.004(2)	−0.001(2)
C(6)	1a	0.1623(8)	−0.2384(6)	0.9411(5)	0.020(3)	0.021(3)	0.018(3)	0.007(2)	0.003(2)	−0.005(2)
Cl(2)	1a	0.3204(2)	−0.3913(2)	1.0031(1)	0.0261(7)	0.0219(7)	0.0367(8)	0.0088(5)	−0.0009(6)	−0.0027(6)
C(7)	1a	0.2147(8)	−0.0954(6)	0.9358(5)	0.017(2)	0.023(3)	0.017(3)	0.004(2)	0.004(2)	−0.002(2)
C(8)	1a	0.1469(4)	0.2748(4)	0.7564(5)	0.022(3)	0.017(2)	0.024(3)	0.000(2)	0.002(2)	−0.005(2)
N(2)	1a	0.2029(4)	0.4336(3)	0.7488(3)	0.012(2)	0.017(2)	0.017(2)	0.004(2)	0.007(2)	−0.006(2)
C(9)	1a	0.1961(4)	0.5421(5)	0.6321(3)	0.022(3)	0.007(2)	0.021(3)	−0.003(2)	−0.004(2)	0.002(2)
C(10)	1a	−0.0148(9)	0.5750(7)	0.5936(5)	0.023(3)	0.030(3)	0.023(3)	0.006(2)	−0.005(2)	0.004(3)
C(11)	1a	0.2885(9)	0.6842(5)	0.6490(5)	0.032(3)	0.013(2)	0.031(3)	−0.006(2)	0.002(2)	−0.005(2)
C(12)	1a	0.323(1)	0.4744(7)	0.5508(5)	0.039(4)	0.034(3)	0.019(3)	−0.002(3)	0.012(3)	−0.004(2)
Cl(3)	1a	0.6337(2)	0.3575(2)	0.8075(1)	0.0148(6)	0.0352(8)	0.0421(9)	0.0073(5)	−0.0043(6)	−0.0111(7)
C(13)	1a	−0.1521(9)	0.4524(6)	0.2061(5)	0.030(3)	0.023(3)	0.018(3)	−0.010(2)	−0.003(2)	0.005(2)
O(2)	1a	−0.2968(7)	0.4352(5)	0.1377(4)	0.050(2)	0.054(3)	0.044(2)	−0.015(2)	−0.005(2)	−0.004(2)
C(14)	1a	−0.1098(8)	0.6135(6)	0.2049(4)	0.026(3)	0.020(3)	0.015(3)	−0.001(2)	0.001(2)	−0.001(2)
C(15)	1a	0.0600(8)	0.6448(6)	0.2498(5)	0.026(3)	0.022(3)	0.021(3)	−0.001(2)	0.003(2)	0.002(2)
C(16)	1a	0.1037(7)	0.7918(6)	0.2443(5)	0.014(2)	0.024(3)	0.021(3)	0.002(2)	0.004(2)	−0.005(2)
Cl(4)	1a	0.3230(2)	0.8262(2)	0.3001(1)	0.0191(6)	0.0291(7)	0.0351(8)	−0.0041(5)	−0.0062(6)	−0.0033(6)
C(17)	1a	−0.0139(6)	0.9156(4)	0.1929(4)	0.013(2)	0.022(3)	0.012(2)	0.003(2)	0.003(2)	−0.003(2)
N(3)	1a	0.0220(5)	1.0622(4)	0.1885(4)	0.018(2)	0.026(2)	0.019(2)	−0.002(2)	0.003(2)	−0.006(2)
C(18)	1a	−0.1901(7)	0.8804(6)	0.1478(5)	0.015(3)	0.025(3)	0.015(3)	0.003(2)	0.004(2)	0.002(2)
Cl(5)	1a	−0.3508(2)	1.0278(2)	0.0879(1)	0.0213(7)	0.0241(7)	0.0337(8)	0.0052(5)	−0.0032(6)	−0.0006(5)
C(19)	1a	−0.2358(8)	0.7337(6)	0.1541(5)	0.014(2)	0.027(3)	0.021(3)	−0.002(2)	−0.001(2)	−0.005(2)
C(20)	1a	−0.1760(4)	0.3655(4)	0.3344(4)	0.022(3)	0.019(2)	0.016(3)	−0.003(2)	0.003(2)	−0.001(2)
N(4)	1a	−0.2253(4)	0.2055(3)	0.3411(3)	0.018(2)	0.021(2)	0.019(2)	−0.002(2)	−0.004(2)	0.001(2)
C(21)	1a	−0.2204(5)	0.0984(6)	0.4582(3)	0.021(3)	0.036(3)	0.014(3)	0.006(2)	0.009(2)	−0.004(2)
C(22)	1a	−0.3402(9)	0.1668(6)	0.5430(5)	0.031(3)	0.026(3)	0.024(3)	0.009(2)	0.004(2)	−0.007(2)
C(23)	1a	−0.012(1)	0.0678(8)	0.4984(6)	0.033(3)	0.035(4)	0.033(4)	0.002(3)	−0.007(3)	0.005(3)
C(24)	1a	−0.308(1)	−0.0436(7)	0.4453(5)	0.039(3)	0.033(3)	0.022(3)	−0.004(3)	0.008(3)	0.001(2)
Cl(6)	1a	−0.6599(2)	0.2807(2)	0.2838(2)	0.0169(7)	0.0324(8)	0.047(1)	0.0003(6)	−0.0021(6)	−0.0040(7)

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References

1. Keck, J.; Krüger, G.; Noll, K.; Machleidt, H.: Synthesen von neuen Amino-Halogen-substituierten Phenylaminoäthanolen. Arzneim.-Forsch. **22** (1972) 861-869.
2. Carpy, A.; Leger, J.-M.; Colleter, J.-C.: Chlorhydrate d'(Amino-4-dichloro-3,5 phényl)-1 *tert*-Butylamino-2-Ethanol (Clenbutérol, NAB-365). Acta Crystallogr. B**36** (1980) 2837-2840.
3. Sheldrick, G. M.: SHELXS-97. Program for the Solution of Crystal Structures. University of Göttingen, Germany 1997.
4. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.