

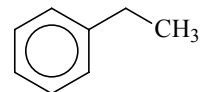
843
MW C_8H_{10}

Ethylbenzene

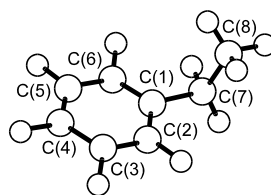
 C_s
(effective symmetry class)

r_s	\AA^a
C(5)–C(6)	1.41(1)
C(4)–C(5)	1.398(3)
C(1)–C(6)	1.375(6)
C(1)–C(7)	1.532(4)
C(7)–C(8)	1.529(4)

θ_s	deg ^{a)}
C(4)–C(5)–C(6)	120.2(5)
C(5)–C(6)–C(1)	119.1(3)
C(6)–C(1)–C(7)	119.0(5)
C(1)–C(7)–C(8)	112.2(3)
C(6)–C(1)–C(2)	122.0(5)
C(3)–C(4)–C(5)	119.3(2)
C(8)–C(7)–C(1)–C(6) ^{b)}	88.7(9)



Atom	a_s [\AA]	b_s [\AA]	c_s [\AA]
C(1)	0.468	0.0	0.320
C(2,6)	−0.182	1.203	0.171
C(3,5)	−1.571	1.206	−0.08
C(4)	−2.2596	0.0	−0.237
C(7)	1.9778	0.0	0.580
C(8)	2.7875	0.0	−0.718



Only one stable conformation was found.

^{a)} Uncertainties derived by error propagation from the standard errors given by the Kraitchman's analysis.

^{b)} Dihedral angle.

Maté, B., Suenram, R.D., Lugez, C.: J. Chem. Phys. **113** (2000) 192.

[II/25D \(3, 2556\)](#)