

1277
MW**C₃H₆O₂****Oxiranemethanol**
2,3-Epoxy-1-propanol
Glycidol**C₁**

r_0	Å	θ_0	deg
C–O (ring)	1.420 ^{a)}	C(1)–C(2)–C(3)	121.2 ^{a)}
C(2)–C(3)	1.466 ^{a)}	H–C(3)–C(2)	116.6 ^{a)}
C(1)–C(2)	1.517 ^{a)}	C(3)–C(2)–H	116.6 ^{a)}
C(1)–O(1)	1.420 ^{a)}	C(2)–C(1)–H ^{b)}	109.47 ^{a)}
C(ring)–H	1.085 ^{a)}	C(2)–C(1)–O(1)	110.5 ^{a)}
O–H	0.960 ^{a)}	C(1)–O(1)–H	106.0 ^{a)}
		H–C(3)–H (ring) ^{c)}	90.0 ^{a)}
		H–C(2)–C(1) (ring) ^{c)}	90.0 ^{a)}
		H bond inner ^{d)}	H bond outer 1 ^{d)}
		O(1)–C(1)–C(2)–C(3)	27(3) (from <i>syn</i>) 141(3) (from <i>syn</i>)
		H–O(1)–C(1)–C(2)	47(5) (from <i>syn</i>) –55(5) (from <i>syn</i>)
		O(1)–C(1)–C(2)–O(2)	41.5 (from <i>syn</i>) ^{e)} –72.5 (from <i>syn</i>) ^{e)}

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
H (hydroxyl) of H bond inner	1.011	1.132	0.633
H (hydroxyl) of H bond outer 1	1.584	1.163	0.304

Two conformers were detected: the H bond inner form is more stable than the H bond outer 1 form by 3.6(4) kJ mol^{–1}.

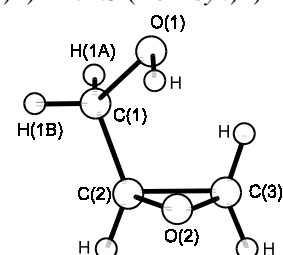
^{a)} Assumed.

^{b)} Atoms assumed to be arranged tetrahedrally around C(1).

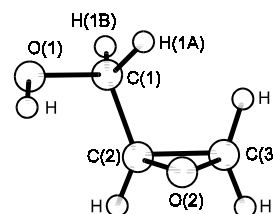
^{c)} Dihedral angle between the plane of the epoxy ring and the adjacent atoms.

^{d)} Uncertainties are estimated to represent three standard deviations.

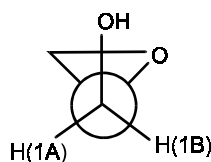
^{e)} This dependent parameter has been calculated from the fitted structure.



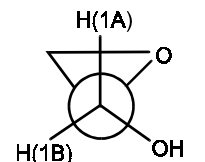
H bond inner



H bond outer 1



H bond inner



H bond outer 1

Marstokk, K.-M., Møllendal, H., Stenstrøm, Y.: Acta Chem. Scand. **46** (1992) 432.