

Species Tag:	76011	Name:	C3H8O2 I
Version:	1		1,3 propanediol,
Date:	March 2010		v = 0,1
Contributor:	B.J. Drouin		Conformer I
Lines Listed:	21811	Q(300.0)=	150865.3530
Freq. (GHz) <	300	Q(225.0)=	105552.4007
Max. J:	30	Q(150.0)=	62153.3312
LOGSTR0=	-10.0	Q(75.00)=	23440.6022
LOGSTR1=	-10.0	Q(37.50)=	8381.8380
Isotope Corr.:	0.0	Q(18.75)=	2967.4252
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	1051.5690
μ_a =	2.917	A=	7701.2351
μ_b =	1.465	B=	3891.2952
μ_c =	1.024	C=	2854.5575

The data set used is from D. F. Plusquellic et al. J. Phys. Chem. A 2009, 113, 12911-12918. The partition function was calculated with a summation over predicted energy levels up to $J = 250$. This value is 20% smaller than that suggested in the cited work which assumed a rigid rotor.