





Bosutinib, ring bonds, 108 conformations (1, 2)(1, 6)(6, 7)(6, 5)(5, 4)(4, 3)(3, 2)(28, 29) (28, 33)(33, 32)(32, 31)(31, 30)(30, 29) (5, 10)(10, 9)(9, 8)(8, 7)(14, 15)(14, 19)(19, 18)(18, 17)(17, 16)(16, 15)1.0 1.1 1.2 1.5 1.3 1.4 1.6

Bond order