Home / QM Descriptor

QM Descriptor

Enter a molecule or reaction SMILES

NC(=O)OC(Cn1ncnn1)c1ccccc1Cl

Draw | SUBMIT | CLEAR RESULTS

Click to select columns to display

DOWNLOAD

Select Columns: Dipole Moment (debye) | IP (hartree) | Sheilding Constant (ppm)

smiles	3D Visualization	dipole moment (debye)	IP (hartree)	shielding constant (ppm)
NC(=O)OC(Cn1ncnn1)c1ccccc1Cl		3.1142127794462215	0.35015110344855654	[193.50969426664514, 46.61887984422171, 70.0582835807637, 183.53292731095854, 125.12157007898581, 146.19712785696996, -5.027879947949666, -47.21106859949474, 48.81197760393699, -77.17407196176677, -113.43188894600628, 59.001808383899444, 68.22415280467051, 69.53666571222867, 71.50765932952824, 68.3063318064934, 57.936302706131585, 781.197488385369, 28.275924837840147, 28.275924837840147, 27.799892807751554, 29.011757265947445, 29.011757265947445, 24.457907791647834, 24.598694705929468, 24.691654549536064, 24.691654549536064, 24.723022308630426]

Click for 3D visualization

Items per page: 10 | 1-1 of 1

3D Visualization

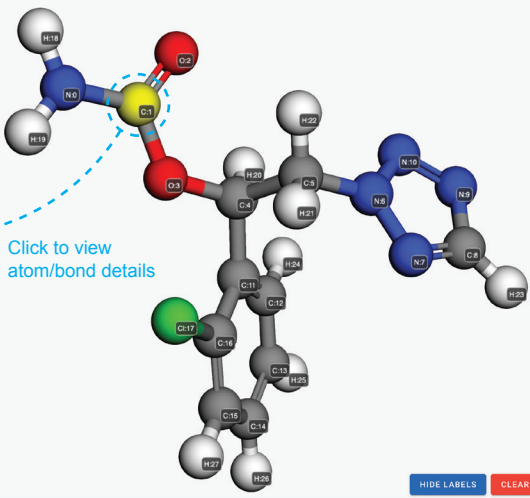
Atom Details

index	1
elem	C
npa charge (e)	1.0122666741068564
npa charge + (e)	0.9649549140942367
npa charge - (e)	0.9680945029474893
npa parr function + (e)	0.019311050657141886
npa parr function - (e)	-0.024648043891251626
shielding constant (ppm)	46.61887984422171
1s valence orbital occupancy (e)	0.0001101484041761136
2s valence orbital occupancy (e)	0.6715836847028376
2p valence orbital occupancy (e)	2.275167046094646
3s valence orbital occupancy (e)	0.00001936758887081911 8
3p valence orbital occupancy (e)	-0.00003621488100996467
4s valence orbital occupancy (e)	0.00002178538163373749 3
4p valence orbital occupancy (e)	0.00005066639904077463

Bond Details

C:1 - N:0 bond

C:1 - O:2 bond



Click to view atom/bond details

HIDE LABELS | CLEAR SELECTED

CLOSE