Spectral method	EI-MS
Scan range	40-550
Sample introduction method	liquid injection
Mass calibration method	PFTBA
Single compound or mixture	single compound
Gas type	He
Notes	70 eV
Ionization mode	positive
Mass measurement	nominal
Instrument type	quadrupole
Chromatography type	GC
Tune type	auto-tune
Instrument make and model	Agilent 5973
Method and software used in data processing	averaged and background subtracted, ACD/SpecManager version 12.01
Chromatographic method	column: DB-5MS (30 m x 0.25 mm x 0.25 um), split ratio: 50:1, injection port temperature: 300°C, temperature ramp: 40°C (hold 1 min) to 300°C (hold 9 min) at 10°C/min; 300°C to 325°C at 15°C/min (hold 5 min), Retention Time: 17.11 min

Submitted Name	2C-C		
Synonyms	4-chloro-2,5-dimethoxyphenethylamine, 2,5-dimethoxy-4-chlorophenethylamine		
Submitter name	Peter Stout	***Submitter facility***	RTI
Acquisition date	2011, 2012	***Standard source***	Grace lot # 658-4104
Standard original phase	solid	***Class***	phenethylamine, hallucinogen
Submitter email	pstout@rti.org		

Formula	$C_{10}H_{14}ClNO_2$	***FW***	215.6767		
InChI	InChI=1/C10H14ClNO2/c1-13-9-6-8(11)10(14-2)5-7(9)3-4-12/h5-6H,3-4,12H2,1-2H3				
SMILES	COc1cc(CCN)c(cc1Cl)OC			***InChI Key***	CGKQFIWIPSIVAS-UHFFFAOYAM
Molar Refractivity	57.58±0.3 cm^3	***Molar Volume***	185.8±3.0 cm^3	***Parachor***	462.1±4.0 cm^3
Index of Refraction	1.531±0.02	***Surface Tension***	38.1±3.0 dyne/cm	***Density***	1.160±0.06 g/cm^3
Dielectric Constant	cannot calculate	***Polarizability***	22.83±0.5 $10^{24}cm^3$	***Monoisotopic Mass***	215.071306 Da
Nominal Mass	215 Da	***Average Mass***	215.6767 Da	***M+***	215.070758 Da
M-	215.071855 Da	***[M+H]+***	216.078583 Da	***[M+H]-***	216.07968 Da
[M-H]+	214.062933 Da	***[M-H]-***	214.06403 Da	***pKa_{IF}***	L
pKa_1	HL/H+L 9.37 (+/-0.10)