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: 15.12 min

Submitted Name	2C-H HCl	***Synonyms***	2,5-dimethoxyphenethylamine		
Submitter name	Peter Stout	***Submitter facility***	RTI	***Acquisition date***	2012
Standard source	Lipomed lot 728.1B2.2L2			***Standard original phase***	solid
Class	phenethylamine	***Submitter email***	pstout@rti.org		

Formula	$C_{10}H_{15}NO_2$	***FW***	181.2316		
InChI	InChI=1/C10H15NO2/c1-12-9-3-4-10(13-2)8(7-9)5-6-11/h3-4,7H,5-6,11H2,1-2H3				
SMILES	COc1ccc(cc1CCN)OC			***InChI Key***	WNCUVUUEJZEATP-UHFFFAOYAJ
Molar Refractivity	52.69±0.3 cm^3	***Molar Volume***	173.9±3.0 cm^3	***Parachor***	426.2±4.0 cm^3
Index of Refraction	1.517±0.02	***Surface Tension***	36.0±3.0 dyne/cm	***Density***	1.041±0.06 g/cm^3
Dielectric Constant	cannot calculate	***Polarizability***	20.88±0.5 $10^{-24}cm^3$	***Monoisotopic Mass***	181.110279 Da
Nominal Mass	181 Da	***Average Mass***	181.2316 Da	***M+***	181.10973 Da
M-	181.110827 Da	***[M+H]+***	182.117555 Da	***[M+H]-***	182.118652 Da
[M-H]+	180.101905 Da	***[M-H]-***	180.103002 Da	***pKa_{IF}***	L
pKa_1	HL/H+L 9.72 (+/-0.10)