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: 16.41 min

Submitted Name	2C-E		
Synonyms	2,5-dimethoxy-4-ethylphenethylamine, 1-(2,5-Dimethoxy-4-ethylphenyl)-2-aminoethane, Europa		
Submitter name	Peter Stout	***Submitter facility***	RTI
Acquisition date	2011, 2012	***Standard source***	Grace lot # 0611000281
Standard original phase	solid	***Class***	phenethylamine, hallucinogen
Submitter email	pstout@rti.org		

Formula	$C_{12}H_{19}NO_2$	***FW***	209.2848		
InChI	InChI=1/C12H19NO2/c1-4-9-7-12(15-3)10(5-6-13)8-11(9)14-2/h7-8H,4-6,13H2,1-3H3				
SMILES	COc1cc(CC)c(cc1CCN)OC			***InChI Key***	VDRGNAMREYBIHA-UHFFFAOYAI
Molar Refractivity	62.24±0.3 cm^3	***Molar Volume***	206.7±3.0 cm^3	***Parachor***	502.8±4.0 cm^3
Index of Refraction	1.514±0.02	***Surface Tension***	34.9±3.0 dyne/cm	***Density***	1.012±0.06 g/cm^3
Dielectric Constant	cannot calculate	***Polarizability***	24.67±0.5 $10^{24}cm^3$	***Monoisotopic Mass***	209.141579 Da
Nominal Mass	209 Da	***Average Mass***	209.2848 Da	***M+***	209.14103 Da
M-	209.142127 Da	***[M+H]+***	210.148855 Da	***[M+H]-***	210.149952 Da
[M-H]+	208.133205 Da	***[M-H]-***	208.134302 Da	***pKa_{IF}***	L
pKa_1	HL/H+L 9.73 (+/-0.10)