

Spectral method	FTIR	Scan range	400-4000 cm ⁻¹
Sample introduction method	ATR diamond single bounce		
Single compound or mixture	single compound	Instrument make and model	Thermo-Nicolet 6700
Spectral resolution	4 cm ⁻¹	Make and model of sampling accessory	OMNIC Smart Orbit
Number of scans co-added	32 scans	Method and software used in data processing	OMNIC version 7.3
Sample introduction phase	liquid		

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
Index of Refraction	1.531±0.02	Surface Tension	38.1±3.0 dyne/cm
Dielectric Constant	cannot calculate	Polarizability	22.83±0.5 10 ²⁴ cm ³
Nominal Mass	215 Da	Average Mass	215.6767 Da
M-	215.071855 Da	[M+H]⁺	216.078583 Da
[M-H]⁺	214.062933 Da	[M-H]⁻	214.06403 Da
pKa_f	HL/H+L 9.37 (+/-0.10)		
		M⁺	215.070758 Da
		[M+H]⁻	216.07968 Da
		pKa_f	L

