25 Jun 2013

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-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)