Yasuda-Shedlovsky Result

Sample name:	**CS000095**	Experiment start time:	**31/07/2011 11:38:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31005_CS000095_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.32	±0.02	8.09	-236.9960	0.9995	0.172 M	25.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-31005 Points 66 to 103	27.61 %	Up	pH-metric	65.8	37.3 M	0.181 M	27.1°C	☑	2.92
11G-31005 Points 34 to 65	37.43 %	Up	pH-metric	61.8	31.5 M	0.174 M	26.0°C	☑	2.77
11G-31005 Points 3 to 33	48.64 %	Up	pH-metric	57.2	25.2 M	0.162 M	24.5°C	☑	2.54

Graphs

Sample name:	**CS000095**	Experiment start time:	**31/07/2011 11:38:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31005_CS000095_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11G-31005 Points 3 to 33

Sample

CS000095 concentration factor	1.000
Base pKa 1	2.54

Sample graphs

Other graphs

Sample name:	**CS000095**	Experiment start time:	**31/07/2011 11:38:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31005_CS000095_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11G-31005 Points 34 to 65

Sample

CS000095 concentration factor 1.000
Base pKa 1 2.77

Sample graphs

Other graphs

Sample name:	**CS000095**	Experiment start time:	**31/07/2011 11:38:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-31005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-31005_CS000095_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11G-31005 Points 66 to 103

Sample

CS000095 concentration factor	1.000
Base pKa 1	2.92

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000095		
Sample by	Weight	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
Sample weight	0.000740 g		
Formula weight	369.40 g/mol		
Solubility	Unknown	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
Molecular weight	369.40		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
pKa 1	4.00		
logp (XH +)	-10.00	31/07/2011 10:48:23	E:\T3 DATA\1107\11G-14012_CS000038_pH-metric psKa.t3r
logP (neutral X)	-10.00		