Yasuda-Shedlovsky Result

Sample name:	**cs000142**	Experiment start time:	**24/08/2011 20:05:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24014_cs000142_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	5.12	±0.00	9.23	-185.4248	1.0000	0.171 M	25.8°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-24014 Points 77 to 120	38.48 %	Up	pH-metric	61.1	30.8 M	0.177 M	26.7°C	☑	4.71
11H-24014 Points 37 to 76	50.94 %	Up	pH-metric	55.6	23.9 M	0.173 M	25.9°C	☑	4.52
11H-24014 Points 3 to 36	65.35 %	Up	pH-metric	49.1	16.3 M	0.163 M	24.7°C	☑	4.24

Graphs

Sample name:	**cs000142**	Experiment start time:	**24/08/2011 20:05:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24014_cs000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-24014 Points 3 to 36

Sample

cs000142 concentration factor	0.888
Base pKa 1	4.24

Sample graphs

Other graphs

Sample name:	**cs000142**	Experiment start time:	**24/08/2011 20:05:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24014_cs000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-24014 Points 37 to 76

Sample

cs000142 concentration factor	0.793
Base pKa 1	4.52

Sample graphs

Other graphs

Sample name:	**cs000142**	Experiment start time:	**24/08/2011 20:05:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24014_cs000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-24014 Points 77 to 120

Sample

cs000142 concentration factor	0.759
Base pKa 1	4.71

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000142	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r
Sample by	Weight	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r
Sample weight	0.000670 g		
Formula weight	295.30 g/mol	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r
Solubility	Unknown	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r
Molecular weight	295.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r

Sample name:	**cs000142**	Experiment start time:	**24/08/2011 20:05:43**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24014_cs000142_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
pKa 1	4.00	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r
logp (XH +)	-10.00	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r
logP (neutral X)	-10.00	24/08/2011 20:05:24	E:\T3 DATA\1108\11H-24012_cs000142_pH-metric psKa.t3r