Yasuda-Shedlovsky Result

Sample name:	**CS000085**	Experiment start time:	**20/08/2011 17:52:32**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20015_CS000085_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	2.99	±0.03	6.79	-158.6773	0.9975	0.174 M	28.5°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-20015 Points 68 to 108	28.03 %	Up	pH-metric	64.9	37.0 M	0.183 M	29.5°C	☑	2.78
11H-20015 Points 34 to 67	39.87 %	Up	pH-metric	59.8	30.0 M	0.176 M	28.7°C	☑	2.64
11H-20015 Points 3 to 33	54.57 %	Up	pH-metric	53.5	21.9 M	0.164 M	27.4°C	☑	2.48

Graphs

Sample name:	**CS000085**	Experiment start time:	**20/08/2011 17:52:32**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20015_CS000085_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-20015 Points 3 to 33

Sample

CS000085 concentration factor	1.000
Base pKa 1	2.48

Sample graphs

Other graphs

Sample name:	**CS000085**	Experiment start time:	**20/08/2011 17:52:32**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20015_CS000085_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-20015 Points 34 to 67

Sample

CS000085 concentration factor	1.000
Base pKa 1	2.64

Sample graphs

Other graphs

Sample name:	**CS000085**	Experiment start time:	**20/08/2011 17:52:32**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20015_CS000085_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-20015 Points 68 to 108

Sample

CS000085 concentration factor	1.000
Base pKa 1	2.78

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000085		
Sample by	Weight	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample weight	0.000820 g		
Formula weight	337.34 g/mol		
Solubility	Unknown	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	337.34		
Individual pKa ionic environments	No		
Number of pKas	1	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r

Sample name:	**CS000085**	Experiment start time:	**20/08/2011 17:52:32**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-20015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-20015_CS000085_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH +)	-10.00	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	20/08/2011 14:03:54	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r