Yasuda-Shedlovsky Result

Sample name:	**CS00064**	Experiment start time:	**02/08/2011 16:38:22**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-02009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-02009-1_CS00064_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.42	±0.09	41.45	-2732.3572	0.9899	0.186 M	28.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-02009 Points 78 to 123	24.32 %	Up	pH-metric	76.1	42.8 M	0.194 M	28.5°C	☑	3.92
11H-02009 Points 38 to 77	31.82 %	Up	pH-metric	75.7	38.8 M	0.188 M	28.2°C	☑	3.73
11H-02009 Points 3 to 37	41.22 %	Up	pH-metric	75.0	33.7 M	0.176 M	27.6°C	☑	3.52

Graphs

Sample name:	**CS00064**	Experiment start time:	**02/08/2011 16:38:22**
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Filename:	**E:\T3 DATA\1107\11H-02009-1_CS00064_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-02009 Points 3 to 37 Quality: Good

Sample

CS00064 concentration factor	1.000
Base pKa 1	3.52

Sample graphs

Other graphs

Sample name:	**CS00064**	Experiment start time:	**02/08/2011 16:38:22**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-02009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-02009-1_CS00064_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-02009 Points 38 to 77 Quality: Good

Sample

CS00064 concentration factor	1.000
Base pKa 1	3.73

Sample graphs

Other graphs

Sample name:	**CS00064**	Experiment start time:	**02/08/2011 16:38:22**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-02009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11H-02009-1_CS00064_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-02009 Points 78 to 123 Quality: Good

Sample

CS00064 concentration factor	1.000
Base pKa 1	3.92

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS00064		
Sample by	Weight		
Sample weight	0.000300 g		
Formula weight	329.38 g/mol		
Solubility	Unknown		
Molecular weight	329.38		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	4.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		