Yasuda-Shedlovsky Result

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 20:17:39**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28012_CS000142_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	4.96	±0.06	23.17	-1271.0600	0.9781	0.182 M	28.8°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-28012 Points 78 to 114	22.95 %	Up	pH-metric	75.9	43.5 M	0.190 M	29.1°C	☑	4.81
11H-28012 Points 38 to 77	30.17 %	Up	pH-metric	75.6	39.7 M	0.183 M	28.9°C	☑	4.74
11H-28012 Points 3 to 37	38.60 %	Up	pH-metric	75.0	35.1 M	0.172 M	28.5°C	☑	4.69

Graphs

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 20:17:39**
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Filename:	**E:\T3 DATA\1108\11H-28012_CS000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-28012 Points 3 to 37

Sample

CS000142 concentration factor	0.833
Base pKa 1	4.69

Sample graphs

Other graphs

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 20:17:39**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28012_CS000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-28012 Points 38 to 77

Sample

CS000142 concentration factor	0.847
Base pKa 1	4.74

Sample graphs

Other graphs

Sample name:	**CS000142**	Experiment start time:	**28/08/2011 20:17:39**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28012_CS000142_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-28012 Points 78 to 114

Sample

CS000142 concentration factor	0.896
Base pKa 1	4.81

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000142		
Sample by	Weight		
Sample weight	0.000960 g		
Formula weight	295.30 g/mol		
Solubility	Unknown		
Molecular weight	295.30		
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		