Yasuda-Shedlovsky Result

Sample name:	**CS000140**	Experiment start time:	**28/08/2011 17:57:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28010_CS000140_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.30	±0.12	35.89	-2397.7000	0.9804	0.191 M	27.3°C
Yasuda-Shedlovsky	9.83	±0.22	-5.38	1317.6800	0.8316	0.191 M	27.3°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-28010 Points 90 to 142	25.89 %	Up	pH-metric	76.1	41.9 M	0.198 M	28.1°C	✓	2.80	✓	0.2
11H-28010 Points 44 to 89	34.17 %	Up	pH-metric	75.8	37.6 M	0.194 M	27.4°C	✓	2.64	✓	0.5
11H-28010 Points 3 to 43	44.87 %	Up	pH-metric	75.0	31.8 M	0.182 M	26.4°C	✓	2.42	✓	0.6

Graphs

Sample name:	**CS000140**	Experiment start time:	**28/08/2011 17:57:16**
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Assay ID:	**11H-28010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28010_CS000140_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-28010 Points 3 to 43

Sample

CS000140 concentration factor	1.584
Base pKa 1	2.42
Base pKa 2	10.67

Sample graphs

Other graphs

Sample name:	**CS000140**	Experiment start time:	**28/08/2011 17:57:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28010_CS000140_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-28010 Points 44 to 89

Sample

CS000140 concentration factor	1.655
Base pKa 1	2.64
Base pKa 2	10.50

Sample graphs

Other graphs

Sample name:	**CS000140**	Experiment start time:	**28/08/2011 17:57:16**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-28010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-28010_CS000140_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-28010 Points 90 to 142

Sample

CS000140 concentration factor	1.498
Base pKa 1	2.80
Base pKa 2	10.25

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000140		
Sample by	Weight		
Sample weight	0.001020 g		
Formula weight	376.46 g/mol		
Solubility	Unknown		
Molecular weight	376.46		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base		
pKa 1	4.00		
pKa 2	10.30		
logP (XH2 2+)	-10.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		