Yasuda-Shedlovsky Result

Sample name:	**cs000115**	Experiment start time:	**22/08/2011 12:07:46**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22006_cs000115_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	1.97	±0.19	4.45	-57.7076	0.7347	0.178 M	26.9°C
Yasuda-Shedlovsky	10.67	±0.03	12.35	5.1132	0.5135	0.178 M	26.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-22006 Points 65 to 99	34.10 %	Up	pH-metric	62.7	33.4 M	0.187 M	27.9°C	☑	1.95	☑	0.9
11H-22006 Points 33 to 64	47.21 %	Up	pH-metric	57.1	25.9 M	0.180 M	26.7°C	☑	2.12	☑	1.0
11H-22006 Points 3 to 32	64.74 %	Up	pH-metric	49.0	16.6 M	0.167 M	26.2°C	☑	2.02	☑	1.2

Graphs

Sample name:	**cs000115**	Experiment start time:	**22/08/2011 12:07:46**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22006_cs000115_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-22006 Points 3 to 32

Sample

cs000115 concentration factor	1.517
Base pKa 1	2.02
Base pKa 2	11.23

Sample graphs

Other graphs

Sample name:	**cs000115**	Experiment start time:	**22/08/2011 12:07:46**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22006_cs000115_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-22006 Points 33 to 64

Sample

cs000115 concentration factor	1.561
Base pKa 1	2.12
Base pKa 2	11.01

Sample graphs

Other graphs

Sample name:	**cs000115**	Experiment start time:	**22/08/2011 12:07:46**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-22006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-22006_cs000115_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-22006 Points 65 to 99

Sample

cs000115 concentration factor	1.488
Base pKa 1	1.95
Base pKa 2	10.91

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000115		
Sample by	Weight	22/08/2011 10:14:14	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Sample weight	0.000960 g		
Formula weight	297.32 g/mol		
Solubility	Unknown	22/08/2011 10:14:14	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Molecular weight	297.32		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base		
pKa 1	3.50		
pKa 2	9.50		
logP (XH2 2+)	-10.00	22/08/2011 10:14:14	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
logp (XH +)	-10.00		
logP (neutral X)	-10.00		