Yasuda-Shedlovsky Result

Sample name:	**CS000173**	Experiment start time:	**06/09/2011 17:22:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06017_CS000173_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	7.14	±0.07	11.20	-181.7701	0.9949	0.169 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-06017 Points 86 to 126	40.10 %	Up	pH-metric	60.9	29.9 M	0.174 M	25.0°C	☑	6.73
11I-06017 Points 44 to 85	52.16 %	Up	pH-metric	55.3	23.2 M	0.171 M	25.0°C	☑	6.58
11I-06017 Points 3 to 43	64.66 %	Up	pH-metric	49.5	16.7 M	0.163 M	24.7°C	☑	6.29

Graphs

Sample name:	**CS000173**	Experiment start time:	**06/09/2011 17:22:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06017_CS000173_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11I-06017 Points 3 to 43

Sample

CS000173 concentration factor	0.922
Base pKa 1	6.29

Sample graphs

Other graphs

Sample name:	**CS000173**	Experiment start time:	**06/09/2011 17:22:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06017_CS000173_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11I-06017 Points 44 to 85

Sample

CS000173 concentration factor	0.871
Base pKa 1	6.58

Sample graphs

Other graphs

Sample name:	**CS000173**	Experiment start time:	**06/09/2011 17:22:59**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06017_CS000173_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11I-06017 Points 86 to 126

Sample

- CS000173 concentration factor 0.879
- Base pKa 1 6.73

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000173		
Sample by	Weight		
Sample weight	0.001170 g		
Formula weight	361.47 g/mol		
Solubility	Unknown	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	361.47		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	9.65		
logp (XH +)	-10.00	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r