Yasuda-Shedlovsky Result

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 11:11:09**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-07006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07006_CS000189_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.10	±0.04	9.82	-233.5808	0.9990	0.171 M	24.8°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-07006 Points 73 to 110	37.78 %	Up	pH-metric	61.8	31.3 M	0.178 M	25.7°C	☑	4.55
11I-07006 Points 38 to 72	50.32 %	Up	pH-metric	56.3	24.2 M	0.173 M	24.8°C	☑	4.26
11I-07006 Points 3 to 37	64.78 %	Up	pH-metric	49.6	16.6 M	0.163 M	23.9°C	☑	3.90

Graphs

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 11:11:09**
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Assay ID:	**11I-07006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07006_CS000189_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11I-07006 Points 3 to 37

Sample

- CS000189 concentration factor 0.820
- Base pKa 1 3.90

Sample graphs

Other graphs

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 11:11:09**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-07006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07006_CS000189_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11I-07006 Points 38 to 72

Sample

CS000189 concentration factor	0.751
Base pKa 1	4.26

Sample graphs

Other graphs

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 11:11:09**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-07006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07006_CS000189_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11I-07006 Points 73 to 110

Sample

CS000189 concentration factor	0.776
Base pKa 1	4.55

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000189		
Sample by	Weight		
Sample weight	0.000990 g		
Formula weight	295.30 g/mol		
Solubility	Unknown	07/09/2011 10:06:14	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	295.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	07/09/2011 10:06:14	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	4.00	07/09/2011 10:06:14	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logp (XH +)	-10.00	07/09/2011 10:06:14	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00	07/09/2011 10:06:14	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r