Yasuda-Shedlovsky Result

Sample name:	**CS000173**	Experiment start time:	**03/09/2011 17:49:38**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-03010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-03010_CS000173_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	6.72	±0.04	20.01	-902.7577	0.9829	0.193 M	26.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-03010 Points 80 to 125	24.16 %	Up	pH-metric	76.8	42.9 M	0.201 M	26.5°C	☑	6.63
11I-03010 Points 40 to 79	32.25 %	Up	pH-metric	76.4	38.6 M	0.196 M	26.1°C	☑	6.59
11I-03010 Points 3 to 39	44.47 %	Up	pH-metric	75.4	32.0 M	0.181 M	25.3°C	☑	6.54

Graphs

Sample name:	**CS000173**	Experiment start time:	**03/09/2011 17:49:38**
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Assay ID:	**11I-03010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-03010_CS000173_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11I-03010 Points 3 to 39

Sample

- CS000173 concentration factor 0.988
- Base pKa 1 6.54

Sample graphs

Other graphs

Sample name:	**CS000173**	Experiment start time:	**03/09/2011 17:49:38**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-03010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-03010_CS000173_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11I-03010 Points 40 to 79

Sample

CS000173 concentration factor	1.028
Base pKa 1	6.59

Sample graphs

Other graphs

Sample name:	**CS000173**	Experiment start time:	**03/09/2011 17:49:38**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-03010**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-03010_CS000173_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11I-03010 Points 80 to 125

Sample

CS000173 concentration factor 1.059
Base pKa 1 6.63

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000173		
Sample by	Weight		
Sample weight	0.001550 g		
Formula weight	361.47 g/mol		
Solubility	Unknown	03/09/2011 10:14:52	E:\T3 DATA\1109\11I-02005_CS000252_Fast UV psKa.t3r
Molecular weight	361.47		
Individual pKa ionic environments	No		
Number of pKas	1	03/09/2011 10:14:52	E:\T3 DATA\1109\11I-02005_CS000252_Fast UV psKa.t3r
Sample is a	Base	03/09/2011 10:14:52	E:\T3 DATA\1109\11I-02005_CS000252_Fast UV psKa.t3r
pKa 1	4.00	03/09/2011 10:14:52	E:\T3 DATA\1109\11I-02005_CS000252_Fast UV psKa.t3r
logp (XH +)	-10.00	03/09/2011 10:14:52	E:\T3 DATA\1109\11I-02005_CS000252_Fast UV psKa.t3r
logP (neutral X)	-10.00	03/09/2011 10:14:52	E:\T3 DATA\1109\11I-02005_CS000252_Fast UV psKa.t3r