Yasuda-Shedlovsky Result

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 10:37:45**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23004**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.66	±0.15	7.01	-126.5516	0.9773	0.160 M	24.0°C
Yasuda-Shedlovsky	6.84	±0.11	8.63	-4.0573	0.0738	0.160 M	24.0°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11G-23004 Points 72 to 110	50.90 %	Up	pH-metric	56.0	23.9 M	0.165 M	24.9°C	☑	3.38	☑	.1
11G-23004 Points 37 to 71	66.82 %	Up	pH-metric	48.5	15.6 M	0.161 M	24.4°C	☑	3.17	☑	.3
11G-23004 Points 3 to 36	72.76 %	Up	pH-metric	46.1	12.7 M	0.154 M	22.6°C	☑	3.20	☑	.4

Graphs

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 10:37:45**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23004**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11G-23004 Points 3 to 36

Sample

CS000041 concentration factor	0.748
Base pKa 1	3.20
Base pKa 2	7.46

Sample graphs

Other graphs

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 10:37:45**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23004**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11G-23004 Points 37 to 71

Sample

CS000041 concentration factor	0.871
Base pKa 1	3.17
Base pKa 2	7.32

Sample graphs

Other graphs

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 10:37:45**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23004**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11G-23004 Points 72 to 110

Sample

CS000041 concentration factor	0.811
Base pKa 1	3.38
Base pKa 2	7.19

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000041	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Sample by	Weight	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Sample weight	0.000350 g		
Formula weight	341.39 g/mol	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Solubility	Unknown	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Molecular weight	341.39		
Individual pKa ionic environments	No		
Number of pKas	2	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
Sample is a	Base		

Sample name:	**CS000041**	Experiment start time:	**23/07/2011 10:37:45**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11G-23004**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
pKa 1	4.00	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
pKa 2	10.00	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
logP (XH2 2+)	-10.00	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
logp (XH +)	-10.00	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r
logP (neutral X)	-10.00	23/07/2011 10:32:22	E:\T3 DATA\1107\11G-22020_CS000041_pH-metric psKa.t3r