Yasuda-Shedlovsky Result

Sample name:	**cs000065**	Experiment start time:	**24/08/2011 12:55:33**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24007_cs000065_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.91	±0.04	11.04	-187.9480	0.9969	0.171 M	24.5°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-24007 Points 81 to 122	28.87 %	Up	pH-metric	65.8	36.5 M	0.177 M	25.5°C	☑	6.62
11H-24007 Points 41 to 80	38.28 %	Up	pH-metric	61.9	31.0 M	0.172 M	24.6°C	☑	6.53
11H-24007 Points 3 to 40	48.08 %	Up	pH-metric	57.8	25.5 M	0.163 M	23.3°C	☑	6.38

Graphs

Sample name:	**cs000065**	Experiment start time:	**24/08/2011 12:55:33**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24007_cs000065_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-24007 Points 3 to 40

Sample

cs000065 concentration factor	1.120
Base pKa 1	6.38

Sample graphs

Other graphs

Sample name:	**cs000065**	Experiment start time:	**24/08/2011 12:55:33**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24007_cs000065_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-24007 Points 41 to 80

Sample

- cs000065 concentration factor 1.056
- Base pKa 1 6.53

Sample graphs

Other graphs

Sample name:	**cs000065**	Experiment start time:	**24/08/2011 12:55:33**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24007**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24007_cs000065_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-24007 Points 81 to 122

Sample

cs000065 concentration factor	1.170
Base pKa 1	6.62

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000065		
Sample by	Weight	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Sample weight	0.000940 g		
Formula weight	475.92 g/mol		
Solubility	Unknown	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Molecular weight	475.92		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	5.60		
logp (XH +)	-10.00	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
logP (neutral X)	-10.00	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r