Yasuda-Shedlovsky Result

Sample name:	**cs000140**	Experiment start time:	**24/08/2011 17:08:35**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24011_cs000140_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.38	±0.00	7.22	-164.1090	1.0000	0.173 M	25.9°C
Yasuda-Shedlovsky	9.68	±0.07	10.22	94.0802	0.9568	0.173 M	25.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-24011 Points 78 to 116	28.51 %	Up	pH-metric	65.7	36.7 M	0.179 M	26.5°C	☑	3.16	☑	).1
11H-24011 Points 39 to 77	37.89 %	Up	pH-metric	61.6	31.2 M	0.174 M	25.9°C	☑	3.06	☑	).2
11H-24011 Points 3 to 38	47.91 %	Up	pH-metric	57.3	25.6 M	0.164 M	25.2°C	☑	2.95	☑	).4

Graphs

Sample name:	**cs000140**	Experiment start time:	**24/08/2011 17:08:35**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24011_cs000140_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-24011 Points 3 to 38

Sample

cs000140 concentration factor	1.186
Base pKa 1	2.95
Base pKa 2	10.46

Sample graphs

Other graphs

Sample name:	**cs000140**	Experiment start time:	**24/08/2011 17:08:35**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24011_cs000140_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-24011 Points 39 to 77

Sample

cs000140 concentration factor	1.277
Base pKa 1	3.06
Base pKa 2	10.22

Sample graphs

Other graphs

Sample name:	**cs000140**	Experiment start time:	**24/08/2011 17:08:35**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24011_cs000140_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-24011 Points 78 to 116

Sample

cs000140 concentration factor	1.262
Base pKa 1	3.16
Base pKa 2	10.10

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000140		
Sample by	Weight	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Sample weight	0.000960 g		
Formula weight	376.46 g/mol		
Solubility	Unknown	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
Molecular weight	376.46		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base		
pKa 1	4.00	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r
pKa 2	Unknown		
logP (XH2 2+)	-10.00	24/08/2011 10:11:44	E:\T3 DATA\1108\11H-01004_DMSO-Blank_pH-metric psKa.t3r

Sample name:	**cs000140**	Experiment start time:	**24/08/2011 17:08:35**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-24011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-24011_cs000140_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
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		