

Protonation constants and thermodynamic properties of amino acid salts for CO₂ capture at high temperatures

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Table 1. Amino acids used in protonation studies.

CAS-No.	Name	Solubility in water g/kg water	Mass fraction purity	Type of amine	Trade name
56-41-7	L-alanine	166.9	≥99.5	Primary	Sigma-Aldrich
56-40-6	Glycine	239	≥99.7	Primary	Sigma-Aldrich
147-85-3	L-proline	1625	≥99	Secondary	Sigma-Aldrich
72-18-4	L-valine	88	≥99.5	Primary	Sigma-Aldrich
2835-81-6	DL-2-aminobutyric acid	210	≥99	Primary	Sigma-Aldrich
62-57-7	2-aminoisobutyric acid	137	≥98	Primary	Sigma-Aldrich
107-97-1	Sarcosine	428	≥98	Secondary	Sigma-Aldrich
327-57-1	L-norleucine	15	≥99	Primary	Sigma-Aldrich
6600-40-4	L-norvaline	107	≥99	Primary	Sigma-Aldrich
107-35-7	Taurine	105	≥99	Primary	Sigma-Aldrich
52-52-8	Cycloleucine	50	≥97	Primary	Sigma-Aldrich

Table 2. Comparison of pK_a of amino acids with published values at 298 K.

Amino acids	Source	pK _a	Method	Medium	Ionic strength(M)
	This work	8.97	Glass electrode	KCl	0.01
Taurine	O'Brien et al. ²⁴	9.06	Glass electrode	KCl	0.01
	Maslowska et al. ²⁵	9.04	Glass electrode	NaClO ₄ /LiClO ₄	0.01
	Datta and Grzybowski ²⁶	8.96	Glass electrode	Other/unknown	0.01
Cycloleucine	This work	9.8	Glass electrode	KCl	0.02
	Israeli et al. ²⁷	9.95	Glass electrode	KNO ₃	0.01
L-alanine	This work	9.678	Glass electrode	KCl	0.02
	Majumdar and Lahiri ²⁸	9.62	Glass electrode	None	0.01
	Dutta and Lahiri ²⁹	9.71	Glass electrode	NaClO ₄ /LiClO ₄	0.01
	Chakravorty and Lahiri ³⁰	9.63	Glass electrode	None	0.01
L-valine	This work	9.57	Glass electrode	KCl	0.02
	Sanaie and Haynes ³¹	9.61	Glass electrode	KNO ₃	0.01
	Majumdar and Lahiri ²⁸	9.57	Glass electrode	NaNO ₃	0.01
	Zhang et al. ³²	9.59	Glass electrode	None	0.01
DL-2-aminobutyric acid	This work	9.731	Glass electrode	KCl	0.02
	Maslowska and Chruscinski ³³	9.75	Glass electrode	NaClO ₄ /LiClO ₄	0.01
	Gergely and Sovago ³⁴	9.77	Glass electrode	KCl	0.01
	Srivastava ³⁵	9.63	Glass electrode	KNO ₃	0.01
L-norleucine	This work	9.46	Glass electrode	KCl	0.02
	Sovago et al. ³⁶	9.81	Glass electrode	KCl	0.01
	Israeli and Pettit ³⁷	9.8	Glass electrode	KNO ₃	0.01
	Gergely and Sovago ³⁸	9.78	Glass electrode	KCl	0.01
Glycine	This work	9.52	Glass electrode	KCl	0.02
	Monajjemi et al. ³⁹	9.69	Spectrophotometry	MeOH mixed	0.01

				solvents	
	Wada et al. ⁴⁰	9.53	Ion selective electrode	Dioxan mixed solvents	0.01
	Jozefonvicz et al. ⁴¹	9.31	Glass electrode	Other mixed solvent	0.01
L-proline	This work	10.39	Glass electrode	KCl	0.02
	El-Sherif ⁴²	10.65	Glass electrode	NaNO ₃	0.01
	Chen and Lin ⁴³	10.52	Glass electrode	NaClO ₄ /LiClO ₄	0.01
	Majumdar and Lahiri ²⁸	10.51	Glass electrode	None	0.01
Monoethanol amine	Fernandes et al. ¹³	9.44	Glass electrode	None	N/A

Note: N/A = not applicable

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Table 3. pK_a values of amines as a function of temperatures.

Amino acids												
Temp. (K)	Sarcosine			Cyclololeucine			L-norleucine			L-norvaline		
	pK_a	SD	IS	pK_a	SD	IS	pK_a	SD	IS	pK_a	SD	IS
298	10.28	0.0572	0.02	9.80	0.0225	0.02	9.46	0.0171	0.02	9.48	0.0219	0.02
313	10.11	0.0533	0.02	9.48	0.0173	0.02	9.14	0.0132	0.02	9.16	0.0082	0.02
323	9.87	0.0516	0.02	9.19	0.0095	0.02	8.88	0.0083	0.02	8.88	0.0090	0.02
333	9.76	0.0602	0.02	9.09	0.0284	0.02	8.76	0.0263	0.02	8.76	0.0266	0.02
343	9.55	0.0748	0.02	8.98	0.0236	0.02	8.65	0.0195	0.02	8.70	0.0179	0.02
353	9.44	0.0650	0.02	8.73	0.0292	0.02	8.41	0.0329	0.02	8.37	0.0296	0.02

Amino acids												
Temp. (K)	L-alanine			Valine			DL-2-aminobutyric acid			2-aminoisobutyric acid		
	pK_a	SD	IS	pK_a	SD	IS	pK_a	SD	IS	pK_a	SD	IS
298	9.68	0.0209	0.02	9.57	0.0093	0.02	9.73	0.0159	0.02	9.90	0.0140	0.02
313	9.29	0.0082	0.02	9.12	0.0098	0.02	9.24	0.0107	0.02	9.54	0.0087	0.02
323	8.93	0.0105	0.02	8.81	0.0051	0.02	9.00	0.0086	0.02	9.32	0.0084	0.02
333	8.75	0.0253	0.02	8.60	0.0051	0.02	8.86	0.0077	0.02	9.03	0.0190	0.02
343	8.54	0.0130	0.02	8.49	0.0071	0.02	8.63	0.0106	0.02	8.93	0.0127	0.02
353	8.36	0.0097	0.02	8.24	0.0114	0.02	8.48	0.0196	0.02	8.55	0.0272	0.02

Amino acids										Amine		
Temp. (K)	Taurine			Glycine			L-proline			Temp.(K)	Monoethanolamine ¹³ (as a benchmark)	
	pK_a	SD	IS	pK_a	SD	IS	pK_a	SD	IS		pK_a	SD
298	8.97	0.0201	0.01	9.52	0.0105	0.02	10.38	0.0225	0.02	288	9.67	0.01
313	8.63	0.0608	0.01	9.14	0.0083	0.02	10.01	0.0187	0.02	298	9.44	0.01
323	8.26	0.0731	0.01	8.87	0.0058	0.02	9.78	0.0106	0.02	308	9.21	0.04
333	8.06	0.0803	0.01	8.71	0.0132	0.02	9.57	0.0129	0.02	318	8.96	0.03
343	8.54	0.0130	0.02	8.49	0.0071	0.02	8.63	0.0106	0.02			
353	8.36	0.0097	0.02	8.24	0.0114	0.02	8.48	0.0196	0.02			

Note: IS = ionic strength; SD = standard deviation

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Table 4. ΔH_m^0 , ΔS_m^0 and ΔG_m^0 values of protonation reaction of amino acids at 298 K and 353 K.

Amino acids /amine	ΔH_m^0 (kJ/mol)	ΔS_m^0 (J/(K•mol))	ΔG_m^0 (kJ/mol) (298K)	ΔG_m^0 (kJ/mol) (353K)
Sarcosine	-31.92	90.51	-58.90	-63.88
2-aminoisobutyric acid	-46.02	36.11	-56.69	-58.37
Cycloleucine	-37.75	60.68	-55.85	-59.18
DL-2-aminoisobutyric acid	-45.02	34.14	-55.20	-57.08
L-alanine	-48.96	20.82	-55.17	-56.31
Valine	-47.74	22.27	-54.38	-55.61
L-norvaline	-38.16	53.29	-54.05	-56.98
L-norleucine	-37.22	56.01	-53.92	-57.00
Taurine	-51.18	0.60	-51.36	-51.40
Glycine	-48.68	19.58	-54.52	-55.59
L-proline	-45.14	47.58	-59.33	-61.94
Monoethanolamine ¹³ (as a benchmark)	-41	42	-53.52	-55.83

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