2-Aminopropionic acid

Other names:	(R)-(-)-alanine (R)-2-aminopropanoic acid (S)-2-Aminopropanoic acid (S)-Alanine 2-Aminopropanoic acid 2-Aminopropanoic acid, L- ALPHA-ALANINE ALPHA-AMINOPROPIONIC ACID Ala Alanine, L- D-2-aminopropanoic acid D-alanine L-(+)-Alanine L-2-Aminopropanoic acid L-2-Aminopropionic acid L-ALANINE L-CH3CH(NH2)COOH L-«alpha»-Alanine L-«alpha»-Aminopropionic acid NSC 206315 Propanoic acid, 2-amino- Propanoic acid, 2-amino-, (S)- Ritalanine alanine propanoic acid, D-2-amino- «alpha»-Alanine «alpha»-Aminopropionic acid
Inchi:	InChI=1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)/t2-/m1/s1
InchiKey:	QNAYBMKLOCPYGJ-UWTATZPHSA-N
Formula:	C3H7NO2
SMILES:	CC(N)C(=O)O
Mol. weight [g/mol]:	89.09
CAS:	56-41-7

Physical Properties

Property code	Value	Unit	Source

af	0.6256		Cheméo Relay (1.0)
hf	-430.26	kJ/mol	Cheméo Relay (1.0)
hfus	10.89	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Cheméo Relay (1.0)
ie	8.96	eV	Cheméo Relay (1.0)
log10ws	0.27		Aqueous Solubility Prediction Method
logp	-0.582		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
tb	460.96	K	Cheméo Relay (1.0)
tc	649.27	K	Cheméo Relay (1.0)
tf	555.82	K	Aqueous Solubility Prediction Method
vc	0.250	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.30	J/mol×K	486.18	Joback Method
cpg	157.40	J/mol×K	518.13	Joback Method
cpg	163.22	J/mol×K	550.08	Joback Method
cpg	168.75	J/mol×K	582.03	Joback Method
cpg	174.01	J/mol×K	613.98	Joback Method
cpg	179.00	J/mol×K	645.93	Joback Method
cpg	183.73	J/mol×K	677.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C302727&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Temperature Dependences and Enthalpic Discrimination of Homochiral Pairwise Interactions of Six a-Amino Acid Enantiomers in Pure Water:	https://www.doi.org/10.1021/je500825a
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1465
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Activity coefficients of glycine, d-alanine and l-valine in aqueous solutions containing MgSO4 at 298.15 K; experimental determination and correlation:	https://www.doi.org/10.1016/j.fluid.2011.10.015

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume