Propanoic acid, 3-amino-2-methyl-

Other names:	.alpha.-methyl-.beta.-alanine
	.beta.-aminoisobutyric acid
	2-(aminomethyl)propionic acid
	2-methyl-.beta.-alanine
	2-methyl-3-aminopropionic acid
	3-Amino-2-methylpropanoic acid
	3-amino-2-methylpropionic acid
	3-aminoisobutyric acid
	DL-Beta-aminoisobutyric acid
	dl-3-Amino-2-methylpropionic acid
	dl-3-Aminoisobutyric acid
	dl-«beta»-Aminoisobutyric acid
	«beta»-Aminoisobutyric acid
Inchi:	InChI=1S/C4H9NO2/c1-3(2-5)4(6)7/h3H,2,5H2,1H3,(H,6,7)
InchiKey:	QCHPKSFMDHPSNR-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CC(CN)C(=O)O
Mol. weight [g/mol]:	103.12
CAS:	10569-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-218.93	kJ/mol	Joback Method
hf	-362.19	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	0.21		Crippen Method
logp	-0.334		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	509.06	K	Joback Method
tc	698.51	K	Joback Method
tf	313.85	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.62	J/mol×K	509.06	Joback Method
cpg	197.96	J/mol×K	540.64	Joback Method
cpg	204.95	J/mol×K	572.21	Joback Method
cpg	211.60	J/mol×K	603.79	Joback Method
cpg	217.92	J/mol×K	635.36	Joback Method
cpg	223.92	J/mol×K	666.94	Joback Method
cpg	229.60	J/mol×K	698.51	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10569729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Binary Diffusion Coefficients of Aqueous Phenylalanine, Tyrosine Isomers, and Aminobutyric Acids at Infinitesimal Concentration and Temperatures from (293.2 to 333.2) K:	https://www.doi.org/10.1021/je3012698

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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