«alpha»-Aminoisobutanoic acid

Other names:	.alpha.-aminoisobutanoic acid
	.alpha.-aminoisobutyric acid
	2-amino-2-methylpropanoic acid
	2-amino-2-methylpropionic acid
	2-aminoisobutyric acid
	2-methylalanine
	AIB
	NSC 16590
	Propionic acid, 2-amino-2-methyl-
	alanine, 2-methyl-
	aminoisobutyric acid
	propanoic acid, 2-amino-2-methyl-
	«alpha»,«alpha»-Dimethylglycine
	«alpha»-Aminoisobutyric acid
	«alpha»-Methylalanine
Inchi:	InChI=1S/C4H9NO2/c1-4(2,5)3(6)7/h5H2,1-2H3,(H,6,7)
InchiKey:	FUOOLUPWFVMBKG-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CC(C)(N)C(=O)O
Mol. weight [g/mol]:	103.12
CAS:	62-57-7

Physical Properties

Property code	Value	Unit	Source
chs	-2330.00 ± 2.00	kJ/mol	NIST Webbook
chs	-2265.99 ± 0.42	kJ/mol	NIST Webbook
gf	-213.65	kJ/mol	Joback Method
hf	-365.66	kJ/mol	Joback Method
hfs	-527.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-594.28 ± 0.48	kJ/mol	NIST Webbook
hfus	9.59	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.192		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	5320.16	kPa	Joback Method
tb	506.27	K	Joback Method

tc	703.19	K	Joback Method
tf	331.27	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.88	J/mol×K	604.73	Joback Method
cpg	222.24	J/mol×K	637.55	Joback Method
cpg	228.19	J/mol×K	670.37	Joback Method
cpg	194.06	J/mol×K	506.27	Joback Method
cpg	201.81	J/mol×K	539.09	Joback Method
cpg	209.08	J/mol×K	571.91	Joback Method
cpg	233.76	J/mol×K	703.19	Joback Method
hsubt	125.80	kJ/mol	450.50	NIST Webbook
hsubt	134.20	kJ/mol	413.50	NIST Webbook
hsubt	129.50 ± 0.40	kJ/mol	455.00	NIST Webbook

Sources

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
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=C62577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hsubt:	Enthalpy of sublimation at a given temperature
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