

DL-Beta-aminoisobutyric acid

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-3-Amino-2-methylpropionic acid dl-3-Aminoisobutyric acid dl-«beta»-Aminoisobutyric acid propanoic acid, 3-amino-2-methyl- «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

Physical Properties

Property code	Value	Unit	Source
af	0.6456		Cheméo Relay (1.0)
chs	-2590.00 ± 1.40	kJ/mol	NIST Webbook
hf	-458.47	kJ/mol	Cheméo Relay (1.0)
hfs	-269.00 ± 1.60	kJ/mol	NIST Webbook
hfus	13.48	kJ/mol	Joback Method
hvap	71.76	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	0.66		Cheméo Relay (1.0)
logp	-0.334		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	480.84	K	Cheméo Relay (1.0)
tc	667.89	K	Cheméo Relay (1.0)
tf	347.82	K	Cheméo Relay (1.0)
vc	0.287	m3/kmol	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10569729&Units=SI

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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