dl-2-Aminobutyric acid

Other names:	(±)-2-aminobutyric acid
	2-Aminobutyric acid
	2-Aminobutyric acid, dl
	Aminobutyric acid,-2-
	Butanoic acid, 2-amino-
	Butanoic acid, 2-amino-, (.+/-.)-
	Butyric acid, 2-amino-, DL-
	Butyric acid, dl-2-amino-, beta-form
	Butyrine
	DL-2-Aminobutanoic acid
	NSC 3251
	alpha-Aminobutyric acid
	dl-2-Amino-n-butyric acid
	dl-«alpha»-Amino-n-butyric acid
	«alpha»-Aminobutyric acid
Inchi:	InChI=1S/C4H9NO2/c1-2-3(5)4(6)7/h3H,2,5H2,1H3,(H,6,7)
InchiKey:	QWCKQJZIFLGMSD-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CCC(N)C(=O)O
Mol. weight [g/mol]:	103.12
CAS:	2835-81-6

Physical Properties

Property code	Value	Unit	Source
chs	-2254.00 ± 1.10	kJ/mol	NIST Webbook
gf	-218.93	kJ/mol	Joback Method
hf	-362.19	kJ/mol	Joback Method
hfs	-605.80 ± 1.10	kJ/mol	NIST Webbook
hfus	13.48	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	0.31		Aqueous Solubility Prediction Method
logp	-0.192		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
hsubt	132.00	kJ/mol	409.00	NIST Webbook
hsubt	132.00 ± 2.00	kJ/mol	409.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2835816&Units=SI

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