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

Physical Properties

Property code	Value	Unit	Source
hf	-452.96	kJ/mol	Cheméo Relay (1.0)
hfus	13.48	kJ/mol	Joback Method
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	0.31		Aqueous Solubility Prediction Method
logp	-0.192		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
tb	475.77	K	Cheméo Relay (1.0)
tf	478.79	K	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

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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