dl-3-Aminoisobutyric acid, methyl ester

Other names: Methyl 3-amino-2-methylpropanoate
Inchi: InChI=1S/C5H11NO2/c1-4(3-6)5(7)8-2/h4H,3,6H2,1-2H3
InchiKey: BXGDNKQFNQZCLG-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: COC(=O)C(C)CN
Mol. weight [g/mol]: 117.15

Physical Properties

Property code	Value	Unit	Source
gf	-178.69	kJ/mol	Joback Method
hf	-362.82	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	-0.246		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	902.20		NIST Webbook
tb	462.18	K	Joback Method
tc	659.06	K	Joback Method
tf	286.53	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.74	J/mol×K	462.18	Joback Method
cpg	220.39	J/mol×K	494.99	Joback Method
cpg	229.66	J/mol×K	527.81	Joback Method
cpg	238.56	J/mol×K	560.62	Joback Method
cpg	247.09	J/mol×K	593.43	Joback Method
cpg	255.24	J/mol×K	626.24	Joback Method
cpg	263.02	J/mol×K	659.06	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U332881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume