D-2-Aminobutyric acid, N-methyl-, methyl ester

Other names: Methyl (2S)-2-(methylamino)butanoate
Inchi: InChI=1S/C6H13NO2/c1-4-5(7-2)6(8)9-3/h5,7H,4H2,1-3H3
InchiKey: INBBIXRVEUBDRU-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CCC(NC)C(=O)OC
Mol. weight [g/mol]: 131.17

Physical Properties

Property code	Value	Unit	Source
gf	-147.33	kJ/mol	Joback Method
hf	-363.78	kJ/mol	Joback Method
hfus	15.66	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.157		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	900.40		NIST Webbook
rinpol	900.40		NIST Webbook
tb	462.70	K	Joback Method
tc	648.02	K	Joback Method
tf	267.20	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.24	J/mol×K	462.70	Joback Method
cpg	252.18	J/mol×K	493.59	Joback Method
cpg	262.71	J/mol×K	524.47	Joback Method
cpg	272.83	J/mol×K	555.36	Joback Method
cpg	282.54	J/mol×K	586.25	Joback Method
cpg	291.85	J/mol×K	617.13	Joback Method
cpg	300.75	J/mol×K	648.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332991&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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