Methyl 1-aminocyclopropanecarboxylate

Other names: 1-Aminocyclopropanecarboxylic acid, methyl ester
Inchi: InChI=1S/C5H9NO2/c1-8-4(7)5(6)2-3-5/h2-3,6H2,1H3
InchiKey: CSHMCEYIMFSLSS-UHFFFAOYSA-N
Formula: C5H9NO2
SMILES: COC(=O)C1(N)CC1
Mol. weight [g/mol]: 115.13
CAS: 72784-42-0

Physical Properties

Property code	Value	Unit	Source
gf	-120.99	kJ/mol	Joback Method
hf	-269.50	kJ/mol	Joback Method
hfus	8.53	kJ/mol	Joback Method
hvap	45.28	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	-0.349		Crippen Method
mcvol	87.870	ml/mol	McGowan Method
pc	4959.33	kPa	Joback Method
rinpol	903.70		NIST Webbook
rinpol	903.70		NIST Webbook
tb	469.60	K	Joback Method
tc	687.04	K	Joback Method
tf	343.37	K	Joback Method
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.45	J/mol×K	469.60	Joback Method
cpg	205.62	J/mol×K	505.84	Joback Method
cpg	214.95	J/mol×K	542.08	Joback Method
cpg	223.55	J/mol×K	578.32	Joback Method
cpg	231.54	J/mol×K	614.56	Joback Method
cpg	239.03	J/mol×K	650.80	Joback Method

cpg	246.13	J/mol×K	687.04	Joback Method

Sources

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=C72784420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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