DL-3-Aminoisobutyric acid, N-dimethylaminomethylene-, ethyl ester

Inchi: InChI=1S/C9H18N2O2/c1-5-13-9(12)8(2)6-10-7-11(3)4/h7-8H,5-6H2,1-4H3
InchiKey: MMQUJTWGIZSXTC-UHFFFAOYSA-N
Formula: C9H18N2O2
SMILES: CCOC(=O)C(C)CN=CN(C)C
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
hf	-329.42	kJ/mol	Joback Method
hvap	49.75	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.775		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1312.00		NIST Webbook
rinpol	1312.00		NIST Webbook
tb	570.29	K	Joback Method
tc	762.15	K	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=U375502&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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