L-Alanyl-L-norleucine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C13H25N3O3/c1-6-7-8-11(13(18)19-5)15-12(17)10(2)14-9-16(3)4/h9-11H,6-8H

InchiKey: LTWGEQCCLPMMFZ-UHFFFAOYSA-N

Formula: C13H25N3O3

SMILES: CCCCC(NC(=O)C(C)N=CN(C)C)C(=O)OC

Mol. weight [g/mol]: 271.36

Physical Properties

Property code	Value	Unit	Source
hf	-476.37	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	0.813		Crippen Method
mcvol	228.680	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1931.00		NIST Webbook
tb	765.41	K	Joback Method
tc	961.80	K	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375958&Units=SI

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