Glycyl-L-valine, N-dimethylaminomethylene-, methyl ester

Inchi: InChI=1S/C11H21N3O3/c1-8(2)10(11(16)17-5)13-9(15)6-12-7-14(3)4/h7-8,10H,6H2,1-5H

InchiKey: BBWXAHALLOGTQX-UHFFFAOYSA-N

Formula: C11H21N3O3

SMILES: COC(=O)C(NC(=O)CN=CN(C)C)C(C)C

Mol. weight [g/mol]: 243.30

Physical Properties

Property code	Value	Unit	Source
hf	-435.09	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	-0.110		Crippen Method
mcvol	200.500	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
tb	719.65	K	Joback Method
tc	918.59	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=U375721&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