5-Aminovaleric acid, N-dimethylaminomethylene-, butyl ester

Inchi: InChI=1S/C12H24N2O2/c1-4-5-10-16-12(15)8-6-7-9-13-11-14(2)3/h11H,4-10H2,1-3H3

InchiKey: FBKSWWRVYYHHHL-UHFFFAOYSA-N

Formula: C12H24N2O2

SMILES: CCCCOC(=O)CCCCN=CN(C)C

Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
hf	-386.06	kJ/mol	Joback Method
hvap	56.82	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.090		Crippen Method
mcvol	203.040	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1678.00		NIST Webbook
tb	639.37	K	Joback Method
tc	822.15	K	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=U375795&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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