

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

Inchi: InChI=1S/C10H20N2O2/c1-4-14-10(13)7-5-6-8-11-9-12(2)3/h9H,4-8H2,1-3H3
InchiKey: IHLHOVNHKIYDNF-UHFFFAOYSA-N
Formula: C10H20N2O2
SMILES: CCOC(=O)CCCCN=CN(C)C
Mol. weight [g/mol]: 200.28

Physical Properties

Property code	Value	Unit	Source
hf	-344.78	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.310		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook
tb	593.61	K	Joback Method
tc	779.73	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375796&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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>

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

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