

L-Alanine, N-dimethylaminomethylene-, ethyl ester

Inchi:	InChI=1S/C8H16N2O2/c1-5-12-8(11)7(2)9-6-10(3)4/h6-7H,5H2,1-4H3
InchiKey:	YHWZFIMLMMNBKB-UHFFFAOYSA-N
Formula:	C8H16N2O2
SMILES:	CCOC(=O)C(C)N=CN(C)C
Mol. weight [g/mol]:	172.22

Physical Properties

Property code	Value	Unit	Source
hf	-308.78	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	0.528		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1229.00		NIST Webbook
tb	547.41	K	Joback Method
tc	741.73	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375641&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

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