

Glycyl-L-norleucine, N-dimethylaminomethylene-, ethyl ester

Inchi:	lnChI=1S/C13H25N3O3/c1-5-7-8-11(13(18)19-6-2)15-12(17)9-14-10-16(3)4/h10-11H,5-9
InchiKey:	VBAUUBVZAQWFDZ-UHFFFAOYSA-N
Formula:	C13H25N3O3
SMILES:	CCCC(C(=O)N(C)C)=CN=CNC(=O)OCC
Mol. weight [g/mol]:	271.36

Physical Properties

Property code	Value	Unit	Source
hf	-471.09	kJ/mol	Joback Method
hvap	71.84	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	0.814		Crippen Method
mcvol	228.680	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1980.00		NIST Webbook
tb	765.85	K	Joback Method
tc	959.87	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=U375960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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