

Gly-Leu, N-dimethylaminomethylene-, methyl ester

Inchi:	InChI=1S/C12H23N3O3/c1-9(2)6-10(12(17)18-5)14-11(16)7-13-8-15(3)4/h8-10H,6-7H2,1
InchiKey:	LGDU CGWCEIRDII-UHFFFAOYSA-N
Formula:	C12H23N3O3
SMILES:	COC(=O)C(CC(C)C)NC(=O)CN=CN(C)C
Mol. weight [g/mol]:	257.33

Physical Properties

Property code	Value	Unit	Source
hf	-455.73	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.280		Crippen Method
mcvol	214.590	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinsol	1921.00		NIST Webbook
rinsol	1921.00		NIST Webbook
tb	742.53	K	Joback Method
tc	939.94	K	Joback Method

Sources

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=U375720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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