L-Glutamine, N,N'-bis(dimethylaminomethylene)-, methyl ester

Inchi: InChI=1S/C12H22N4O3/c1-15(2)8-13-10(12(18)19-5)6-7-11(17)14-9-16(3)4/h8-10H,6-7H

InchiKey: AMCDWFIVEDQBPB-UHFFFAOYSA-N

Formula: C12H22N4O3

SMILES: COC(=O)C(CCC(=O)N=CN(C)C)N=CN(C)C

Mol. weight [g/mol]: 270.33

Physical Properties

Property code	Value	Unit	Source
hf	-354.17	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-0.05		Crippen Method
logp	0.015		Crippen Method
mcvol	220.270	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook
tb	781.92	K	Joback Method
tc	986.07	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=U375612&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