Glycine, N-(m-toluoy)-, methyl esterl

Inchi: InChI=1S/C11H13NO3/c1-8-4-3-5-9(6-8)11(14)12-7-10(13)15-2/h3-6H,7H2,1-2H3,(H,12,
InchiKey: DIOHBBQCUZSFKL-UHFFFAOYSA-N
Formula: C11H13NO3
SMILES: COC(=O)CN=C(O)c1cccc(C)c1
Mol. weight [g/mol]: 207.23

Physical Properties

Property code	Value	Unit	Source
hf	-369.91	kJ/mol	Joback Method
hvap	72.25	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.473		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1772.00		NIST Webbook
tb	727.77	K	Joback Method
tc	940.78	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299638&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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