

L-Alanine, N-(m-toluoyl)-, methyl ester

Inchi:	InChI=1S/C12H15NO3/c1-8-5-4-6-10(7-8)11(14)13-9(2)12(15)16-3/h4-7,9H,1-3H3,(H,13
InchiKey:	LEBSCEMDKLYKTO-UHFFFAOYSA-N
Formula:	C12H15NO3
SMILES:	COC(=O)C(C)N=C(O)c1cccc(C)c1
Mol. weight [g/mol]:	221.25

Physical Properties

Property code	Value	Unit	Source
hf	-395.83	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.861		Crippen Method
mcpvol	175.170	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	750.21	K	Joback Method
tc	963.94	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=U299637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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