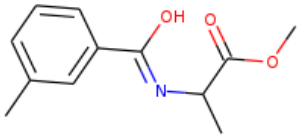
l-Alanine, N-(m-toluoyl)-, methyl ester

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,13,14)
InChI Key: LEBSCEMDKLYKTO-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: COC(=O)C(C)N=C(O)c1cccc(C)c1
Molecular Weight: 221.25



Physical Properties

Property	Value	Unit	Source
$\Delta_f H°_{gas}$	-395.83	kJ/mol	Joback Method
$\Delta_{vap} H°$	74.09	kJ/mol	Joback Method
$logP_{oct/wat}$	1.86		Crippen Method
P_c	2480.12	kPa	Joback Method
T_{boil}	750.21	K	Joback Method
T_c	963.94	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/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,13,14)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$logP_{oct/wat}$: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).

T_c: Critical Temperature (K).