

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

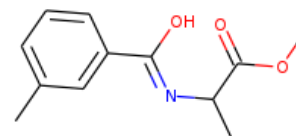
InChI: InChI=1S/C12H15NO3/c1-8-5-4-6-10(7-8)11(14)13-9(2)12(15)16-3/h4-7,9H,1-3H3,(H,13,14)

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
$\Delta_f H^\circ_{\text{gas}}$	-395.83	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	74.09	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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,\(H,13,14\)](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/ci9903071>

Legend

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

Latest version available from:

<https://www.cheméo.com/cid/85-533-6/l-Alanine%2C%20N-%28m-toluoyl%29-%2C%20methyl%20ester>

Generated by Cheméo on Wed, 14 Apr 2021 11:28:01 +0000.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.