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

Inchi: InChI=1S/C12H15NO3/c1-8-4-6-10(7-5-8)11(14)13-9(2)12(15)16-3/h4-7,9H,1-3H3,(H,13
InchiKey: CTLUSWRBHZCLEM-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: COC(=O)C(C)NC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 221.25

Physical Properties

Property code	Value	Unit	Source
gf	-122.95	kJ/mol	Joback Method
hf	-375.14	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.286		Crippen Method
mcvol	175.170	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook
tb	685.51	K	Joback Method
tc	902.99	K	Joback Method
tf	423.69	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.51	J/mol×K	685.51	Joback Method
cpg	476.01	J/mol×K	721.76	Joback Method
cpg	488.60	J/mol×K	758.00	Joback Method
cpg	500.31	J/mol×K	794.25	Joback Method
cpg	511.14	J/mol×K	830.49	Joback Method
cpg	521.12	J/mol×K	866.74	Joback Method
cpg	530.27	J/mol×K	902.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299646&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume