Glycinic acid, n-2-tert-butyl-phenyl-, ethyl ester

Inchi: InChI=1S/C14H21NO2/c1-5-17-13(16)10-15-12-9-7-6-8-11(12)14(2,3)4/h6-9,15H,5,10H2

InchiKey: YVCLTTINPMKQGL-UHFFFAOYSA-N

Formula: C14H21NO2

SMILES: CCOC(=O)CNc1ccccc1C(C)(C)C

Mol. weight [g/mol]: 235.32

Physical Properties

Property code	Value	Unit	Source
gf	28.09	kJ/mol	Joback Method
hf	-307.31	kJ/mol	Joback Method
hfus	26.14	kJ/mol	Joback Method
hvap	63.99	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.959		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
tb	674.61	K	Joback Method
tc	886.29	K	Joback Method
tf	413.72	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.82	J/mol×K	674.61	Joback Method
cpg	568.04	J/mol×K	709.89	Joback Method
cpg	583.22	J/mol×K	745.17	Joback Method
cpg	597.39	J/mol×K	780.45	Joback Method
cpg	610.61	J/mol×K	815.73	Joback Method
cpg	622.92	J/mol×K	851.01	Joback Method
cpg	634.36	J/mol×K	886.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009260&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume