ethyl 3-phenyl-DL-alaninate

Inchi: InChI=1S/C11H15NO2/c1-3-14-11(13)9(2)12-10-7-5-4-6-8-10/h4-9,12H,3H2,1-2H3
InchiKey: FMFDWCAQDWISCD-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCOC(=O)C(C)Nc1ccccc1
Mol. weight [g/mol]: 193.24
CAS: 1795-96-6

Physical Properties

Property code	Value	Unit	Source
gf	7.18	kJ/mol	Joback Method
hf	-230.45	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.050		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	603.78	K	Joback Method
tc	817.31	K	Joback Method
tf	349.97	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.75	J/mol×K	603.78	Joback Method
cpg	411.36	J/mol×K	639.37	Joback Method
cpg	425.07	J/mol×K	674.96	Joback Method
cpg	437.92	J/mol×K	710.54	Joback Method
cpg	449.93	J/mol×K	746.13	Joback Method
cpg	461.11	J/mol×K	781.72	Joback Method
cpg	471.50	J/mol×K	817.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795966&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

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