Glycine, N-phenyl-, ethyl ester

Other names:	Ethyl phenylglycinate
	Ethyl N-phenylglycinate
	N-Phenylglycine ethyl ester
Inchi:	InChI=1S/C10H13NO2/c1-2-13-10(12)8-11-9-6-4-3-5-7-9/h3-7,11H,2,8H2,1H3
InchiKey:	MLSGRWDEDYJNER-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCOC(=O)CNc1ccccc1
Mol. weight [g/mol]:	179.22
CAS:	2216-92-4

Physical Properties

Property code	Value	Unit	Source
gf	1.20	kJ/mol	Joback Method
hf	-204.53	kJ/mol	Joback Method
hfus	23.58	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.662		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	546.70	K	NIST Webbook
tc	794.04	K	Joback Method
tf	353.70	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.22	J/mol×K	581.34	Joback Method
cpg	361.78	J/mol×K	616.79	Joback Method
cpg	374.53	J/mol×K	652.24	Joback Method
cpg	386.49	J/mol×K	687.69	Joback Method
cpg	397.69	J/mol×K	723.14	Joback Method
cpg	408.14	J/mol×K	758.59	Joback Method

cpg	417.86	J/mol×K	794.04	Joback Method

Sources

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=C2216924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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