Beta-phenylserine, ethyl ester

Inchi: InChI=1S/C11H15NO3/c1-2-15-11(14)9(12)10(13)8-6-4-3-5-7-8/h3-7,9-10,13H,2,12H2,1
InchiKey: RCUYHYDTFXMONZ-UHFFFAOYSA-N
Formula: C11H15NO3
SMILES: CCOC(=O)C(N)C(O)c1ccccc1
Mol. weight [g/mol]: 209.24
CAS: 40682-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-155.02	kJ/mol	Joback Method
hf	-407.64	kJ/mol	Joback Method
hfus	23.31	kJ/mol	Joback Method
hvap	78.06	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	0.610		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	717.88	K	Joback Method
tc	928.14	K	Joback Method
tf	426.39	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.13	J/mol×K	717.88	Joback Method
cpg	470.77	J/mol×K	752.92	Joback Method
cpg	481.62	J/mol×K	787.97	Joback Method
cpg	491.68	J/mol×K	823.01	Joback Method
cpg	500.99	J/mol×K	858.05	Joback Method
cpg	509.57	J/mol×K	893.10	Joback Method
cpg	517.46	J/mol×K	928.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40682562&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

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