D-Ala, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C14H20N2O3/c1-4-19-14(18)16-11(3)13(17)15-10(2)12-8-6-5-7-9-12/h5-11H,4

InchiKey: LUANQXLMWQRBRW-WDEREUQCSA-N

Formula: C14H20N2O3

SMILES: CCOC(=O)NC(C)C(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-9.53	kJ/mol	Joback Method
hf	-356.76	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	1.998		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1992.00		NIST Webbook
tb	776.02	K	Joback Method
tc	989.95	K	Joback Method
tf	471.37	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.19	J/mol×K	776.02	Joback Method
cpg	637.18	J/mol×K	811.67	Joback Method
cpg	650.12	J/mol×K	847.33	Joback Method
cpg	662.04	J/mol×K	882.98	Joback Method
cpg	672.98	J/mol×K	918.64	Joback Method
cpg	682.98	J/mol×K	954.29	Joback Method
cpg	692.07	J/mol×K	989.95	Joback Method

Sources

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=R587454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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