L-Phenylalanine, N,N-dimethyl-

Other names: Alanine, N,N-dimethyl-3-phenyl-, L-
N,N-Dimethylphenylalanine
Phenylalanine, N,N-dimethyl-
Inchi: InChI=1S/C11H15NO2/c1-12(2)10(11(13)14)8-9-6-4-3-5-7-9/h3-7,10H,8H2,1-2H3,(H,13,
InchiKey: HOGIQTACRLIOHC-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CN(C)C(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]: 193.24
CAS: 17469-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-3.25	kJ/mol	Joback Method
hf	-236.40	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	67.44	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.244		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	635.81	K	Joback Method
tc	834.70	K	Joback Method
tf	368.37	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.86	J/mol×K	635.81	Joback Method
cpg	425.54	J/mol×K	668.96	Joback Method
cpg	437.41	J/mol×K	702.11	Joback Method
cpg	448.52	J/mol×K	735.26	Joback Method

cpg	458.91	J/mol×K	768.40	Joback Method
cpg	468.60	J/mol×K	801.55	Joback Method
cpg	477.66	J/mol×K	834.70	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=C17469895&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
ie:	Ionization energy
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