N-Valylphenylalanine

Inchi: InChI=1S/C14H20N2O3/c1-9(2)12(15)13(17)16-11(14(18)19)8-10-6-4-3-5-7-10/h3-7,9,11
InchiKey: GJNDXQBALKCYSZ-UHFFFAOYSA-N
Formula: C14H20N2O3
SMILES: CC(C)C(N)C(=O)NC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]: 264.32
CAS: 75946-40-6

Physical Properties

Property code	Value	Unit	Source
chs	-7601.70 ± 1.50	kJ/mol	NIST Webbook
gf	-66.73	kJ/mol	Joback Method
hf	-401.73	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hvap	95.12	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	0.782		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	867.70	K	Joback Method
tc	1083.71	K	Joback Method
tf	525.56	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.14	J/mol×K	867.70	Joback Method
cpg	668.39	J/mol×K	903.70	Joback Method
cpg	678.74	J/mol×K	939.70	Joback Method
cpg	688.27	J/mol×K	975.70	Joback Method
cpg	697.02	J/mol×K	1011.71	Joback Method
cpg	705.05	J/mol×K	1047.71	Joback Method
cpg	712.41	J/mol×K	1083.71	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=C75946406&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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