

L-Phenylalanine, N-acetyl-

Other names:

2-acetamido-3-phenylpropanoic acid
Acetyl-L-phenylalanine
Acetylphenylalanine
Alanine, N-acetyl-3-phenyl-, L-
L-N-Acetylphenylalanine
N-Acetyl-L-phenylalanine
N-Acetyl-l-phenalanine
N-Acetylphenylalanine
N-acetyl-3-phenyl-L-alanine
NSC 45699

Inchi:

InChI=1S/C11H13NO3/c1-8(13)12-10(11(14)15)7-9-5-3-2-4-6-9/h2-6,10H,7H2,1H3,(H,12)

InchiKey:

CBQJSKKFNMDLON-JTQLQIEISA-N

Formula:

C11H13NO3

SMILES:

CC(=O)NC(Cc1ccccc1)C(=O)O

Mol. weight [g/mol]:

207.23

CAS:

2018-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-153.56	kJ/mol	Joback Method
hf	-363.04	kJ/mol	Joback Method
hfus	27.15	kJ/mol	Joback Method
hvap	78.57	kJ/mol	Joback Method
log10ws	-1.41		Aqueous Solubility Prediction Method
logp	0.818		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	727.41	K	Joback Method
tc	935.55	K	Joback Method
tf	438.49	K	Joback Method
vc	0.604	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.65	J/molxK	727.41	Joback Method
cpg	448.24	J/molxK	762.10	Joback Method
cpg	458.08	J/molxK	796.79	Joback Method
cpg	467.20	J/molxK	831.48	Joback Method
cpg	475.64	J/molxK	866.17	Joback Method
cpg	483.42	J/molxK	900.86	Joback Method
cpg	490.60	J/molxK	935.55	Joback Method

Sources

Measurements of the solubilities of derivatized amino acids in supercritical carbon dioxide:

<https://www.doi.org/10.1016/j.fluid.2007.01.032>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2018613&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

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