L-Phenylalanine, N-acetyl-, methyl ester

Other names:	Alanine, N-acetyl-3-phenyl-, methyl ester, L- (S)-N-Acetyl-3-phenylalanine methyl ester Acetyl-L-phenylalanine methyl ester Methyl N-acetyl-L-phenylalaninate N-Acetyl-L-phenylalanine methyl ester N-Acetylphenylalanine methyl ester Methyl (S)-2-(acetylamino)-3-phenylpropanoate Methyl N-acetylphenylalaninate
Inchi:	InChI=1S/C12H15NO3/c1-9(14)13-11(12(15)16-2)8-10-6-4-3-5-7-10/h3-7,11H,8H2,1-2H3
InchiKey:	IKGHIFGXPVLPFD-NSHDSACASA-N
Formula:	C12H15NO3
SMILES:	COC(=O)C(Cc1ccccc1)N=C(C)O
Mol. weight [g/mol]:	221.25
CAS:	3618-96-0

Physical Properties

Property code	Value	Unit	Source
hf	-384.36	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.747		Crippen Method
mcvol	175.170	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1714.60		NIST Webbook
rinpol	1714.60		NIST Webbook
tb	745.23	K	Joback Method
tc	958.17	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3618960&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation 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