N-«alpha»-Acetyl lysine, butyl ester

Inchi: InChI=1S/C12H24N2O3/c1-3-4-9-17-12(16)11(14-10(2)15)7-5-6-8-13/h11H,3-9,13H2,1-2
InchiKey: NHFKYFOFZQOTNF-UHFFFAOYSA-N
Formula: C12H24N2O3
SMILES: CCCCOC(=O)C(CCCCN)NC(C)=O
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	-159.28	kJ/mol	Joback Method
hf	-566.41	kJ/mol	Joback Method
hfus	38.00	kJ/mol	Joback Method
hvap	74.90	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	0.963		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	726.38	K	Joback Method
tc	917.70	K	Joback Method
tf	468.01	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.42	J/mol×K	726.38	Joback Method
cpg	625.63	J/mol×K	758.27	Joback Method
cpg	639.03	J/mol×K	790.15	Joback Method
cpg	651.65	J/mol×K	822.04	Joback Method
cpg	663.50	J/mol×K	853.92	Joback Method
cpg	674.59	J/mol×K	885.81	Joback Method
cpg	684.95	J/mol×K	917.70	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=R32026&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
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