Glycine, N-methyl-n-butoxycarbonyl-, hexyl ester

Inchi: InChI=1S/C14H27NO4/c1-4-6-8-9-11-18-13(16)12-15(3)14(17)19-10-7-5-2/h4-12H2,1-3H

InchiKey: QDAZBEMOSIZGHT-UHFFFAOYSA-N

Formula: C14H27NO4

SMILES: CCCCCCOC(=O)CN(C)C(=O)OCCCC

Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	-290.06	kJ/mol	Joback Method
hf	-754.36	kJ/mol	Joback Method
hfus	40.61	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.978		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1753.00		NIST Webbook
tb	684.74	K	Joback Method
tc	860.03	K	Joback Method
tf	424.33	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.28	J/mol×K	684.74	Joback Method
cpg	678.19	J/mol×K	713.95	Joback Method
cpg	693.32	J/mol×K	743.17	Joback Method
cpg	707.69	J/mol×K	772.38	Joback Method
cpg	721.30	J/mol×K	801.60	Joback Method
cpg	734.18	J/mol×K	830.81	Joback Method
cpg	746.33	J/mol×K	860.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320651&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

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