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

Inchi: InChI=1S/C14H27NO4/c1-5-6-9-19-14(17)15(4)11-13(16)18-10-7-8-12(2)3/h12H,5-11H2

InchiKey: IKXXFOCSUVPIOJ-UHFFFAOYSA-N

Formula: C14H27NO4

SMILES: CCCCOC(=O)N(C)CC(=O)OCCCC(C)C

Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	-292.50	kJ/mol	Joback Method
hf	-759.64	kJ/mol	Joback Method
hfus	37.09	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.834		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1714.00		NIST Webbook
tb	684.30	K	Joback Method
tc	861.80	K	Joback Method
tf	409.33	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.75	J/mol×K	684.30	Joback Method
cpg	678.88	J/mol×K	713.88	Joback Method
cpg	694.21	J/mol×K	743.47	Joback Method
cpg	708.76	J/mol×K	773.05	Joback Method
cpg	722.52	J/mol×K	802.63	Joback Method
cpg	735.52	J/mol×K	832.22	Joback Method
cpg	747.76	J/mol×K	861.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320650&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