Glycine, N-methyl-N-ethoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C12H23NO4/c1-5-16-12(15)13(4)9-11(14)17-8-6-7-10(2)3/h10H,5-9H2,1-4H3
InchiKey: QQPPHEBQJVKMNB-UHFFFAOYSA-N
Formula: C12H23NO4
SMILES: CCOC(=O)N(C)CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
gf	-309.34	kJ/mol	Joback Method
hf	-718.36	kJ/mol	Joback Method
hfus	31.91	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	2.054		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
tb	638.54	K	Joback Method
tc	817.39	K	Joback Method
tf	386.79	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.86	J/mol×K	638.54	Joback Method
cpg	570.04	J/mol×K	668.35	Joback Method
cpg	584.50	J/mol×K	698.16	Joback Method
cpg	598.26	J/mol×K	727.96	Joback Method
cpg	611.30	J/mol×K	757.77	Joback Method
cpg	623.65	J/mol×K	787.58	Joback Method
cpg	635.31	J/mol×K	817.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320675&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

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