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

Inchi: InChI=1S/C13H25NO4/c1-5-8-18-13(16)14(4)10-12(15)17-9-6-7-11(2)3/h11H,5-10H2,1-4

InchiKey: OROPMVJNLFNQTJ-UHFFFAOYSA-N

Formula: C13H25NO4

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

Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-300.92	kJ/mol	Joback Method
hf	-739.00	kJ/mol	Joback Method
hfus	34.50	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.444		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	661.42	K	Joback Method
tc	839.39	K	Joback Method
tf	398.06	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.15	J/mol×K	661.42	Joback Method
cpg	623.83	J/mol×K	691.08	Joback Method
cpg	638.75	J/mol×K	720.74	Joback Method
cpg	652.92	J/mol×K	750.41	Joback Method
cpg	666.35	J/mol×K	780.07	Joback Method
cpg	679.05	J/mol×K	809.73	Joback Method
cpg	691.02	J/mol×K	839.39	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=U320623&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