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

Inchi: InChI=1S/C13H25NO4/c1-4-6-7-8-10-17-12(15)11-14(3)13(16)18-9-5-2/h4-11H2,1-3H3
InchiKey: ABITVDVGJFPEQZ-UHFFFAOYSA-N
Formula: C13H25NO4
SMILES: CCCCCCOC(=O)CN(C)C(=O)OCCC
Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-298.48	kJ/mol	Joback Method
hf	-733.72	kJ/mol	Joback Method
hfus	38.02	kJ/mol	Joback Method
hvap	64.89	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.588		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1678.00		NIST Webbook
tb	661.86	K	Joback Method
tc	837.37	K	Joback Method
tf	413.06	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.70	J/mol×K	661.86	Joback Method
cpg	623.13	J/mol×K	691.11	Joback Method
cpg	637.83	J/mol×K	720.36	Joback Method
cpg	651.80	J/mol×K	749.62	Joback Method
cpg	665.07	J/mol×K	778.87	Joback Method
cpg	677.63	J/mol×K	808.12	Joback Method
cpg	689.49	J/mol×K	837.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320624&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