Glycine, N-methyl-N-ethoxycarbonyl-, hexyl ester

Inchi: InChI=1S/C12H23NO4/c1-4-6-7-8-9-17-11(14)10-13(3)12(15)16-5-2/h4-10H2,1-3H3
InchiKey: SHHNWUGAOCTACQ-UHFFFAOYSA-N
Formula: C12H23NO4
SMILES: CCCCCCOC(=O)CN(C)C(=O)OCC
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
gf	-306.90	kJ/mol	Joback Method
hf	-713.08	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	62.66	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.198		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1596.00		NIST Webbook
tb	638.98	K	Joback Method
tc	815.13	K	Joback Method
tf	401.79	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.43	J/mol×K	638.98	Joback Method
cpg	569.34	J/mol×K	668.34	Joback Method
cpg	583.57	J/mol×K	697.70	Joback Method
cpg	597.11	J/mol×K	727.05	Joback Method
cpg	609.97	J/mol×K	756.41	Joback Method
cpg	622.17	J/mol×K	785.77	Joback Method
cpg	633.70	J/mol×K	815.13	Joback Method

Sources

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=U320676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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