Glycine, N-methyl-N-ethoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C11H21NO4/c1-4-6-7-8-16-10(13)9-12(3)11(14)15-5-2/h4-9H2,1-3H3
InchiKey: QLGSBVZXBUXOOY-UHFFFAOYSA-N
Formula: C11H21NO4
SMILES: CCCCCOC(=O)CN(C)C(=O)OCC
Mol. weight [g/mol]: 231.29

Physical Properties

Property code	Value	Unit	Source
gf	-315.32	kJ/mol	Joback Method
hf	-692.44	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.808		Crippen Method
mcvol	190.710	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1523.00		NIST Webbook
tb	616.10	K	Joback Method
tc	793.24	K	Joback Method
tf	390.52	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.57	J/mol×K	616.10	Joback Method
cpg	516.91	J/mol×K	645.62	Joback Method
cpg	530.61	J/mol×K	675.15	Joback Method
cpg	543.66	J/mol×K	704.67	Joback Method
cpg	556.07	J/mol×K	734.19	Joback Method
cpg	567.86	J/mol×K	763.72	Joback Method
cpg	579.01	J/mol×K	793.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320674&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