Glycine, N-methyl-N-methoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C10H19NO4/c1-4-5-6-7-15-9(12)8-11(2)10(13)14-3/h4-8H2,1-3H3
InchiKey: XGTLVJMKTPZTAM-UHFFFAOYSA-N
Formula: C10H19NO4
SMILES: CCCCCOC(=O)CN(C)C(=O)OC
Mol. weight [g/mol]: 217.26

Physical Properties

Property code	Value	Unit	Source
gf	-323.74	kJ/mol	Joback Method
hf	-671.80	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	58.21	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.418		Crippen Method
mcvol	176.620	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1486.00		NIST Webbook
tb	593.22	K	Joback Method
tc	771.66	K	Joback Method
tf	379.25	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.22	J/mol×K	593.22	Joback Method
cpg	465.93	J/mol×K	622.96	Joback Method
cpg	479.02	J/mol×K	652.70	Joback Method
cpg	491.52	J/mol×K	682.44	Joback Method
cpg	503.42	J/mol×K	712.18	Joback Method
cpg	514.73	J/mol×K	741.92	Joback Method
cpg	525.44	J/mol×K	771.66	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=U320605&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

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