Glycine, N-methyl-N-methoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C11H21NO4/c1-9(2)6-5-7-16-10(13)8-12(3)11(14)15-4/h9H,5-8H2,1-4H3
InchiKey: ZQJJJKGHHWXLOC-UHFFFAOYSA-N
Formula: C11H21NO4
SMILES: COC(=O)N(C)CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 231.29

Physical Properties

Property code	Value	Unit	Source
gf	-317.76	kJ/mol	Joback Method
hf	-697.72	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.664		Crippen Method
mcvol	190.710	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	615.66	K	Joback Method
tc	795.73	K	Joback Method
tf	375.52	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.99	J/mol×K	615.66	Joback Method
cpg	517.61	J/mol×K	645.67	Joback Method
cpg	531.55	J/mol×K	675.68	Joback Method
cpg	544.83	J/mol×K	705.69	Joback Method
cpg	557.43	J/mol×K	735.70	Joback Method
cpg	569.38	J/mol×K	765.72	Joback Method
cpg	580.67	J/mol×K	795.73	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=U320606&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