Glycine, N-methyl-N-ethoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C10H19NO4/c1-5-14-10(13)11(4)6-9(12)15-7-8(2)3/h8H,5-7H2,1-4H3
InchiKey: MJHZIEDRWJWUMJ-UHFFFAOYSA-N
Formula: C10H19NO4
SMILES: CCOC(=O)N(C)CC(=O)OCC(C)C
Mol. weight [g/mol]: 217.26

Physical Properties

Property code	Value	Unit	Source
gf	-326.18	kJ/mol	Joback Method
hf	-677.08	kJ/mol	Joback Method
hfus	26.73	kJ/mol	Joback Method
hvap	57.82	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.274		Crippen Method
mcvol	176.620	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1393.00		NIST Webbook
tb	592.78	K	Joback Method
tc	774.37	K	Joback Method
tf	364.25	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.62	J/mol×K	592.78	Joback Method
cpg	466.61	J/mol×K	623.04	Joback Method
cpg	479.97	J/mol×K	653.31	Joback Method
cpg	492.70	J/mol×K	683.57	Joback Method
cpg	504.80	J/mol×K	713.84	Joback Method
cpg	516.28	J/mol×K	744.10	Joback Method
cpg	527.14	J/mol×K	774.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320672&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