Glycine, N-(3-methyl-1-oxobutyl)-, methyl ester

Other names:	Methyl N-isovalerylglycine
	N-Isovalerylglycine methyl ester
Inchi:	InChI=1S/C8H15NO3/c1-6(2)4-7(10)9-5-8(11)12-3/h6H,4-5H2,1-3H3,(H,9,10)
InchiKey:	SWOIBHOWNKRRFN-UHFFFAOYSA-N
Formula:	C8H15NO3
SMILES:	COC(=O)CNC(=O)CC(C)C
Mol. weight [g/mol]:	173.21
CAS:	56009-37-1

Physical Properties

Property code	Value	Unit	Source
gf	-259.41	kJ/mol	Joback Method
hf	-517.64	kJ/mol	Joback Method
hfus	22.44	kJ/mol	Joback Method
hvap	55.35	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.322		Crippen Method
mcvol	142.570	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1346.40		NIST Webbook
tb	562.33	K	Joback Method
tc	752.51	K	Joback Method
tf	339.67	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.83	J/mol×K	562.33	Joback Method
cpg	358.00	J/mol×K	594.03	Joback Method
cpg	369.61	J/mol×K	625.72	Joback Method
cpg	380.67	J/mol×K	657.42	Joback Method
cpg	391.18	J/mol×K	689.12	Joback Method
cpg	401.15	J/mol×K	720.82	Joback Method

cpg	410.57	J/mol×K	752.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56009371&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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