

Glycine, N-(3-methyl-1-oxo-2-butenyl)-, methyl ester

Other names:	Methyl N-(«beta»-methylcrotonyl)glycine N-(«beta»-Methylcrotonyl)glycine methyl ester «beta»-Methylcrotonylglycine, methyl ester (3-Methyl-but-2-enoylamino)-acetic acid methyl ester
Inchi:	InChI=1S/C8H13NO3/c1-6(2)4-7(10)9-5-8(11)12-3/h4H,5H2,1-3H3,(H,9,10)
InchiKey:	HQJXTLHTVWAWPO-UHFFFAOYSA-N
Formula:	C8H13NO3
SMILES:	COC(=O)CNC(=O)C=C(C)C
Mol. weight [g/mol]:	171.19
CAS:	56009-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-185.30	kJ/mol	Joback Method
hf	-404.93	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.242		Crippen Method
mcvol	138.270	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	566.81	K	Joback Method
tc	764.40	K	Joback Method
tf	335.63	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.75	J/molxK	566.81	Joback Method
cpg	337.24	J/molxK	599.74	Joback Method

cpg	348.16	J/mol×K	632.67	Joback Method
cpg	358.49	J/mol×K	665.60	Joback Method
cpg	368.28	J/mol×K	698.54	Joback Method
cpg	377.52	J/mol×K	731.47	Joback Method
cpg	386.24	J/mol×K	764.40	Joback Method

Sources

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=C56009348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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