Glycine, n-methyl-n-methoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C9H17NO4/c1-7(2)6-14-8(11)5-10(3)9(12)13-4/h7H,5-6H2,1-4H3
InchiKey: BZWVRIAMYUYYOR-UHFFFAOYSA-N
Formula: C9H17NO4
SMILES: COC(=O)N(C)CC(=O)OCC(C)C
Mol. weight [g/mol]: 203.24

Physical Properties

Property code	Value	Unit	Source
af	0.6363		Cheméo Relay (1.0)
hf	-803.63	kJ/mol	Cheméo Relay (1.0)
hfus	24.14	kJ/mol	Joback Method
hvap	67.75	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-0.88		Cheméo Relay (1.0)
logp	0.884		Crippen Method
mcvol	162.530	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1356.00		NIST Webbook
tb	520.32	K	Cheméo Relay (1.0)
tc	685.49	K	Cheméo Relay (1.0)
tf	264.27	K	Cheméo Relay (1.0)
vc	0.619	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.85	J/mol×K	569.90	Joback Method
cpg	417.13	J/mol×K	600.46	Joback Method
cpg	429.82	J/mol×K	631.02	Joback Method
cpg	441.93	J/mol×K	661.58	Joback Method
cpg	453.45	J/mol×K	692.14	Joback Method
cpg	464.40	J/mol×K	722.69	Joback Method
cpg	474.76	J/mol×K	753.25	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320603&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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