Glycine, n-methyl-n-methoxycarbonyl-, butyl ester

Inchi: InChI=1S/C9H17NO4/c1-4-5-6-14-8(11)7-10(2)9(12)13-3/h4-7H2,1-3H3
InchiKey: JTNWHBZXMUFBTK-UHFFFAOYSA-N
Formula: C9H17NO4
SMILES: CCCCOC(=O)CN(C)C(=O)OC
Mol. weight [g/mol]: 203.24

Physical Properties

Property code	Value	Unit	Source
af	0.6677		Cheméo Relay (1.0)
hf	-795.19	kJ/mol	Cheméo Relay (1.0)
hfus	27.66	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-0.97		Cheméo Relay (1.0)
logp	1.028		Crippen Method
mcvol	162.530	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1396.00		NIST Webbook
tb	523.19	K	Cheméo Relay (1.0)
tc	692.19	K	Cheméo Relay (1.0)
tf	246.40	K	Cheméo Relay (1.0)
vc	0.624	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.49	J/mol×K	570.34	Joback Method
cpg	416.47	J/mol×K	600.34	Joback Method
cpg	428.89	J/mol×K	630.34	Joback Method
cpg	440.76	J/mol×K	660.34	Joback Method
cpg	452.08	J/mol×K	690.34	Joback Method
cpg	462.84	J/mol×K	720.34	Joback Method
cpg	473.05	J/mol×K	750.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320604&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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