Glycine, N-methyl-n-butoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C15H29NO4/c1-4-6-8-9-10-12-19-14(17)13-16(3)15(18)20-11-7-5-2/h4-13H2,1

InchiKey: WWBBOBJSVRNBMX-UHFFFAOYSA-N

Formula: C15H29NO4

SMILES: CCCCCCCOC(=O)CN(C)C(=O)OCCCC

Mol. weight [g/mol]: 287.40

Physical Properties

Property code	Value	Unit	Source
gf	-281.64	kJ/mol	Joback Method
hf	-775.00	kJ/mol	Joback Method
hfus	43.20	kJ/mol	Joback Method
hvap	69.34	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.368		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	707.62	K	Joback Method
tc	883.14	K	Joback Method
tf	435.60	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.10	J/mol×K	707.62	Joback Method
cpg	734.44	J/mol×K	736.87	Joback Method
cpg	749.97	J/mol×K	766.13	Joback Method
cpg	764.69	J/mol×K	795.38	Joback Method
cpg	778.63	J/mol×K	824.63	Joback Method
cpg	791.79	J/mol×K	853.89	Joback Method
cpg	804.18	J/mol×K	883.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320652&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