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

Inchi: InChI=1S/C16H31NO4/c1-4-6-8-9-10-11-13-20-15(18)14-17(3)16(19)21-12-7-5-2/h4-14H

InchiKey: QRWSNJSEWYCSGR-UHFFFAOYSA-N

Formula: C16H31NO4

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

Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-273.22	kJ/mol	Joback Method
hf	-795.64	kJ/mol	Joback Method
hfus	45.79	kJ/mol	Joback Method
hvap	71.56	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.759		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	730.50	K	Joback Method
tc	906.76	K	Joback Method
tf	446.87	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.04	J/mol×K	730.50	Joback Method
cpg	791.81	J/mol×K	759.88	Joback Method
cpg	807.71	J/mol×K	789.25	Joback Method
cpg	822.77	J/mol×K	818.63	Joback Method
cpg	836.99	J/mol×K	848.01	Joback Method
cpg	850.41	J/mol×K	877.39	Joback Method
cpg	863.01	J/mol×K	906.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320653&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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