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

Inchi: InChI=1S/C25H49NO4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-22-29-24(27)23-26

InchiKey: GRIPBMCISFNBGA-UHFFFAOYSA-N

Formula: C25H49NO4

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

Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
gf	-197.44	kJ/mol	Joback Method
hf	-981.40	kJ/mol	Joback Method
hfus	69.10	kJ/mol	Joback Method
hvap	91.60	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	7.269		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	803.42	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	936.42	K	Joback Method
tc	1152.27	K	Joback Method
tf	548.30	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.02	J/mol×K	936.42	Joback Method
cpg	1347.09	J/mol×K	972.40	Joback Method
cpg	1366.56	J/mol×K	1008.37	Joback Method
cpg	1384.49	J/mol×K	1044.35	Joback Method
cpg	1400.93	J/mol×K	1080.32	Joback Method
cpg	1415.94	J/mol×K	1116.30	Joback Method
cpg	1429.57	J/mol×K	1152.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320661&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