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

Inchi: InChI=1S/C20H39NO4/c1-4-6-8-9-10-11-12-13-14-15-17-24-19(22)18-21(3)20(23)25-16-

InchiKey: MPDYFOIWIRPHLU-UHFFFAOYSA-N

Formula: C20H39NO4

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

Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
gf	-239.54	kJ/mol	Joback Method
hf	-878.20	kJ/mol	Joback Method
hfus	56.15	kJ/mol	Joback Method
hvap	80.47	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.319		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	822.02	K	Joback Method
tc	1007.51	K	Joback Method
tf	491.95	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.59	J/mol×K	822.02	Joback Method
cpg	1031.01	J/mol×K	852.93	Joback Method
cpg	1048.35	J/mol×K	883.85	Joback Method
cpg	1064.63	J/mol×K	914.76	Joback Method
cpg	1079.87	J/mol×K	945.68	Joback Method
cpg	1094.10	J/mol×K	976.59	Joback Method
cpg	1107.34	J/mol×K	1007.51	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=U320657&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