Glycine, N-methyl-N-ethoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C17H33NO4/c1-4-6-7-8-9-10-11-12-13-14-22-16(19)15-18(3)17(20)21-5-2/h4-1

InchiKey: NEGSXDGHXWZHDD-UHFFFAOYSA-N

Formula: C17H33NO4

SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)OCC

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-264.80	kJ/mol	Joback Method
hf	-816.28	kJ/mol	Joback Method
hfus	48.38	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	4.149		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2026.00		NIST Webbook
tb	753.38	K	Joback Method
tc	930.96	K	Joback Method
tf	458.14	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.05	J/mol×K	753.38	Joback Method
cpg	850.22	J/mol×K	782.98	Joback Method
cpg	866.48	J/mol×K	812.57	Joback Method
cpg	881.85	J/mol×K	842.17	Joback Method
cpg	896.35	J/mol×K	871.76	Joback Method
cpg	909.99	J/mol×K	901.36	Joback Method
cpg	922.78	J/mol×K	930.96	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320681&Units=SI

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