Glycine, N-methyl-N-propoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C21H41NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-18-25-20(23)19-22(3)21(24)2

InchiKey: BEUKTNBMNLKHLY-UHFFFAOYSA-N

Formula: C21H41NO4

SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)OCCC

Mol. weight [g/mol]: 371.56

Physical Properties

Property code	Value	Unit	Source
hf	-1045.62	kJ/mol	Cheméo Relay (1.0)
hfus	58.74	kJ/mol	Joback Method
hvap	111.47	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
log10ws	-5.44		Cheméo Relay (1.0)
logp	5.709		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	628.21	K	Cheméo Relay (1.0)
tc	810.88	K	Cheméo Relay (1.0)
tf	288.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.03	J/mol×K	844.90	Joback Method
cpg	1092.91	J/mol×K	876.51	Joback Method
cpg	1110.63	J/mol×K	908.12	Joback Method
cpg	1127.22	J/mol×K	939.73	Joback Method
cpg	1142.70	J/mol×K	971.34	Joback Method
cpg	1157.10	J/mol×K	1002.95	Joback Method
cpg	1170.46	J/mol×K	1034.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320631&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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