DL-Alanine, N-methyl-N-hexyloxycarbonyl-, decyl ester

Inchi: InChI=1S/C21H41NO4/c1-5-7-9-11-12-13-14-16-17-25-20(23)19(3)22(4)21(24)26-18-15-

InchiKey: SSWQYCXHFBFMDF-UHFFFAOYSA-N

Formula: C21H41NO4

SMILES: CCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCC

Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
gf	-233.56	kJ/mol	Joback Method
hf	-904.12	kJ/mol	Joback Method
hfus	55.22	kJ/mol	Joback Method
hvap	82.31	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.708		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2408.00		NIST Webbook
rinpol	2408.00		NIST Webbook
tb	844.46	K	Joback Method
tc	1034.29	K	Joback Method
tf	488.22	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.49	J/mol×K	844.46	Joback Method
cpg	1093.39	J/mol×K	876.10	Joback Method
cpg	1111.11	J/mol×K	907.74	Joback Method
cpg	1127.68	J/mol×K	939.38	Joback Method
cpg	1143.14	J/mol×K	971.02	Joback Method
cpg	1157.51	J/mol×K	1002.66	Joback Method
cpg	1170.82	J/mol×K	1034.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392639&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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