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

Inchi: InChI=1S/C23H45NO4/c1-5-7-9-11-12-13-14-15-16-18-19-27-22(25)21(3)24(4)23(26)28-

InchiKey: VRUGVCMCKSMXRL-UHFFFAOYSA-N

Formula: C23H45NO4

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

Mol. weight [g/mol]: 399.61

Physical Properties

Property code	Value	Unit	Source
gf	-216.72	kJ/mol	Joback Method
hf	-945.40	kJ/mol	Joback Method
hfus	60.40	kJ/mol	Joback Method
hvap	86.76	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.488		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	890.22	K	Joback Method
tc	1090.37	K	Joback Method
tf	510.76	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.33	J/mol×K	890.22	Joback Method
cpg	1219.15	J/mol×K	923.58	Joback Method
cpg	1237.62	J/mol×K	956.94	Joback Method
cpg	1254.78	J/mol×K	990.30	Joback Method
cpg	1270.65	J/mol×K	1023.65	Joback Method
cpg	1285.29	J/mol×K	1057.01	Joback Method
cpg	1298.73	J/mol×K	1090.37	Joback Method

Sources

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=U392641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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