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

Inchi: InChI=1S/C17H33NO4/c1-5-7-9-11-13-21-16(19)15(3)18(4)17(20)22-14-12-10-8-6-2/h15

InchiKey: YOLAHOPAAGUBQB-UHFFFAOYSA-N

Formula: C17H33NO4

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

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-267.24	kJ/mol	Joback Method
hf	-821.56	kJ/mol	Joback Method
hfus	44.86	kJ/mol	Joback Method
hvap	73.40	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.147		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	752.94	K	Joback Method
tc	931.93	K	Joback Method
tf	443.14	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.53	J/mol×K	752.94	Joback Method
cpg	850.85	J/mol×K	782.77	Joback Method
cpg	867.25	J/mol×K	812.60	Joback Method
cpg	882.72	J/mol×K	842.44	Joback Method
cpg	897.31	J/mol×K	872.27	Joback Method
cpg	911.01	J/mol×K	902.10	Joback Method
cpg	923.84	J/mol×K	931.93	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=U392635&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