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

Inchi: InChI=1S/C18H35NO4/c1-5-7-9-11-13-14-22-17(20)16(3)19(4)18(21)23-15-12-10-8-6-2/l

InchiKey: FNFSEQOEKBCZJE-UHFFFAOYSA-N

Formula: C18H35NO4

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

Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
gf	-258.82	kJ/mol	Joback Method
hf	-842.20	kJ/mol	Joback Method
hfus	47.45	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.537		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
tb	775.82	K	Joback Method
tc	956.46	K	Joback Method
tf	454.41	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.51	J/mol×K	775.82	Joback Method
cpg	910.21	J/mol×K	805.93	Joback Method
cpg	926.92	J/mol×K	836.03	Joback Method
cpg	942.68	J/mol×K	866.14	Joback Method
cpg	957.49	J/mol×K	896.25	Joback Method
cpg	971.38	J/mol×K	926.35	Joback Method
cpg	984.36	J/mol×K	956.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392636&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