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

Inchi: InChI=1S/C16H31NO4/c1-5-7-9-11-13-21-16(19)17(4)14(3)15(18)20-12-10-8-6-2/h14H,5

InchiKey: OORIDIVDADVNAD-UHFFFAOYSA-N

Formula: C16H31NO4

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

Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-275.66	kJ/mol	Joback Method
hf	-800.92	kJ/mol	Joback Method
hfus	42.27	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.757		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	730.06	K	Joback Method
tc	908.02	K	Joback Method
tf	431.87	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.53	J/mol×K	730.06	Joback Method
cpg	792.47	J/mol×K	759.72	Joback Method
cpg	808.53	J/mol×K	789.38	Joback Method
cpg	823.72	J/mol×K	819.04	Joback Method
cpg	838.05	J/mol×K	848.70	Joback Method
cpg	851.55	J/mol×K	878.36	Joback Method
cpg	864.21	J/mol×K	908.02	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=U392634&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