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

Inchi: InChI=1S/C22H43NO4/c1-5-7-9-11-12-13-15-17-19-27-22(25)23(4)20(3)21(24)26-18-16-

InchiKey: KYXMCYMTSPZSPW-UHFFFAOYSA-N

Formula: C22H43NO4

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

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-225.14	kJ/mol	Joback Method
hf	-924.76	kJ/mol	Joback Method
hfus	57.81	kJ/mol	Joback Method
hvap	84.53	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	6.098		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	2483.00		NIST Webbook
rinpol	2483.00		NIST Webbook
tb	867.34	K	Joback Method
tc	1061.87	K	Joback Method
tf	499.49	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.60	J/mol×K	867.34	Joback Method
cpg	1155.94	J/mol×K	899.76	Joback Method
cpg	1174.03	J/mol×K	932.18	Joback Method
cpg	1190.89	J/mol×K	964.60	Joback Method
cpg	1206.56	J/mol×K	997.03	Joback Method
cpg	1221.06	J/mol×K	1029.45	Joback Method
cpg	1234.45	J/mol×K	1061.87	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=U392677&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