DL-Alanine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, nonyl ester

Inchi: InChI=1S/C22H43NO4/c1-6-9-11-12-13-14-15-17-26-21(24)19(4)23(5)22(25)27-18-20(8-
InchiKey: QCVYDUKEFXIONS-UHFFFAOYSA-N
Formula: C22H43NO4
SMILES: CCCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-227.58	kJ/mol	Joback Method
hf	-930.04	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	84.15	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.954		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	866.90	K	Joback Method
tc	1061.39	K	Joback Method
tf	484.49	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.05	J/mol×K	866.90	Joback Method
cpg	1156.38	J/mol×K	899.32	Joback Method
cpg	1174.44	J/mol×K	931.73	Joback Method
cpg	1191.26	J/mol×K	964.15	Joback Method
cpg	1206.88	J/mol×K	996.56	Joback Method
cpg	1221.34	J/mol×K	1028.98	Joback Method
cpg	1234.66	J/mol×K	1061.39	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=U392660&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

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