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

Inchi: InChI=1S/C21H41NO4/c1-7-11-13-18(9-3)15-25-20(23)17(5)22(6)21(24)26-16-19(10-4)1
InchiKey: UMRRJBKAQLMSSH-UHFFFAOYSA-N
Formula: C21H41NO4
SMILES: CCCCC(CC)COC(=O)C(C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
gf	-238.44	kJ/mol	Joback Method
hf	-914.68	kJ/mol	Joback Method
hfus	48.17	kJ/mol	Joback Method
hvap	81.53	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.419		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpol	2243.00		NIST Webbook
rinpol	2243.00		NIST Webbook
tb	843.58	K	Joback Method
tc	1034.17	K	Joback Method
tf	458.22	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.42	J/mol×K	843.58	Joback Method
cpg	1094.38	J/mol×K	875.35	Joback Method
cpg	1112.13	J/mol×K	907.11	Joback Method
cpg	1128.71	J/mol×K	938.88	Joback Method
cpg	1144.15	J/mol×K	970.64	Joback Method
cpg	1158.47	J/mol×K	1002.41	Joback Method
cpg	1171.70	J/mol×K	1034.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392670&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

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