

DL-Alanine, N-methyl-N-(but-4-en-1-yloxycarbonyl)-, tridecyl ester

InChI: InChI=1S/C22H41NO4/c1-5-7-9-10-11-12-13-14-15-16-17-19-26-21(24)20(3)23(4)22(25)
InChIKey: NDGOQDUMAKOZBN-UHFFFAOYSA-N

Formula: C22H41NO4

SMILES: C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCC

Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
gf	-137.30	kJ/mol	Joback Method
hf	-799.33	kJ/mol	Joback Method
hfus	56.53	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.874		Crippen Method
mvol	341.400	ml/mol	McGowan Method
pc	982.69	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	864.02	K	Joback Method
tc	1057.90	K	Joback Method
tf	497.73	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.39	J/molxK	864.02	Joback Method
cpg	1127.16	J/molxK	896.33	Joback Method
cpg	1144.72	J/molxK	928.65	Joback Method
cpg	1161.12	J/molxK	960.96	Joback Method
cpg	1176.38	J/molxK	993.27	Joback Method
cpg	1190.56	J/molxK	1025.58	Joback Method
cpg	1203.67	J/molxK	1057.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392738&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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