

DL-Alanine, N-methyl-N-((1R)-(-)-menthyloxycarbonyl)-, undecyl ester

InChI: InChI=1S/C26H49NO4/c1-7-8-9-10-11-12-13-14-15-18-30-25(28)22(5)27(6)26(29)31-24-
InChIKey: KHNCDUIRDQIRHQ-UHFFFAOYSA-N

Formula: C26H49NO4

SMILES: CCCCCCCCCCOC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
gf	-184.87	kJ/mol	Joback Method
hf	-998.96	kJ/mol	Joback Method
hfus	58.62	kJ/mol	Joback Method
hvap	92.86	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.978		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
pc	830.98	kPa	Joback Method
rinpol	2742.00		NIST Webbook
rinpol	2742.00		NIST Webbook
tb	968.63	K	Joback Method
tc	1186.29	K	Joback Method
tf	528.47	K	Joback Method
vc	1.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.69	J/molxK	968.63	Joback Method
cpg	1415.84	J/molxK	1004.91	Joback Method
cpg	1434.06	J/molxK	1041.18	Joback Method
cpg	1450.37	J/molxK	1077.46	Joback Method
cpg	1464.84	J/molxK	1113.74	Joback Method
cpg	1477.51	J/molxK	1150.02	Joback Method
cpg	1488.41	J/molxK	1186.29	Joback Method

Sources

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=U392798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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