

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

InChI: InChI=1S/C25H47NO4/c1-7-8-9-10-11-12-13-14-17-29-24(27)21(5)26(6)25(28)30-23-18-
InChIKey: YACYAKSBZSQXKG-UHFFFAOYSA-N

Formula: C25H47NO4

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

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
gf	-193.29	kJ/mol	Joback Method
hf	-978.32	kJ/mol	Joback Method
hfus	56.03	kJ/mol	Joback Method
hvap	90.63	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.588		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
pc	878.96	kPa	Joback Method
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	945.75	K	Joback Method
tc	1157.87	K	Joback Method
tf	517.20	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.61	J/mol×K	945.75	Joback Method
cpg	1351.67	J/mol×K	981.10	Joback Method
cpg	1369.90	J/mol×K	1016.46	Joback Method
cpg	1386.35	J/mol×K	1051.81	Joback Method
cpg	1401.06	J/mol×K	1087.16	Joback Method
cpg	1414.05	J/mol×K	1122.52	Joback Method
cpg	1425.39	J/mol×K	1157.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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