

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

InChI: InChI=1S/C27H51NO4/c1-7-8-9-10-11-12-13-14-15-16-19-31-26(29)23(5)28(6)27(30)32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InChIKey: NAGBMYYNVLCGBX-UHFFFAOYSA-N

Formula: C27H51NO4

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

Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
gf	-176.45	kJ/mol	Joback Method
hf	-1019.60	kJ/mol	Joback Method
hfus	61.21	kJ/mol	Joback Method
hvap	95.09	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	7.368		Crippen Method
mcvol	405.290	ml/mol	McGowan Method
pc	786.83	kPa	Joback Method
rinpol	2839.00		NIST Webbook
rinpol	2839.00		NIST Webbook
tb	991.51	K	Joback Method
tc	1215.80	K	Joback Method
tf	539.74	K	Joback Method
vc	1.532	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1460.03	J/molxK	991.51	Joback Method
cpg	1480.31	J/molxK	1028.89	Joback Method
cpg	1498.51	J/molxK	1066.27	Joback Method
cpg	1514.68	J/molxK	1103.66	Joback Method
cpg	1528.88	J/molxK	1141.04	Joback Method
cpg	1541.16	J/molxK	1178.42	Joback Method
cpg	1551.59	J/molxK	1215.80	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=U392799&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
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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