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

Inchi: InChI=1S/C28H53NO4/c1-7-8-9-10-11-12-13-14-15-16-17-20-32-27(30)24(5)29(6)28(31)
InchiKey: VTQZFHBGLQQRRF-UHFFFAOYSA-N
Formula: C28H53NO4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 467.72

Physical Properties

Property code	Value	Unit	Source
gf	-168.03	kJ/mol	Joback Method
hf	-1040.24	kJ/mol	Joback Method
hfus	63.80	kJ/mol	Joback Method
hvap	97.31	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	7.758		Crippen Method
mcvol	419.380	ml/mol	McGowan Method
pc	746.11	kPa	Joback Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook
tb	1014.39	K	Joback Method
tc	1246.48	K	Joback Method
tf	551.01	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1524.59	J/mol×K	1014.39	Joback Method
cpg	1545.01	J/mol×K	1053.07	Joback Method
cpg	1563.20	J/mol×K	1091.75	Joback Method
cpg	1579.20	J/mol×K	1130.44	Joback Method
cpg	1593.10	J/mol×K	1169.12	Joback Method
cpg	1604.95	J/mol×K	1207.80	Joback Method
cpg	1614.81	J/mol×K	1246.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392800&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

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