

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

InChI: InChI=1S/C31H59NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-35-30(33)27(5)3
InChIKey: MNZDEGCJOIHZGV-UHFFFAOYSA-N

Formula: C31H59NO4

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

Mol. weight [g/mol]: 509.80

Physical Properties

Property code	Value	Unit	Source
gf	-142.77	kJ/mol	Joback Method
hf	-1102.16	kJ/mol	Joback Method
hfus	71.57	kJ/mol	Joback Method
hvap	103.99	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	8.929		Crippen Method
mcvol	461.650	ml/mol	McGowan Method
pc	641.25	kPa	Joback Method
rinpol	3244.00		NIST Webbook
rinpol	3244.00		NIST Webbook
tb	1083.03	K	Joback Method
tc	1346.43	K	Joback Method
tf	584.82	K	Joback Method
vc	1.756	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1719.15	J/molxK	1083.03	Joback Method
cpg	1740.12	J/molxK	1126.93	Joback Method
cpg	1758.20	J/molxK	1170.83	Joback Method
cpg	1773.51	J/molxK	1214.73	Joback Method
cpg	1786.14	J/molxK	1258.63	Joback Method
cpg	1796.22	J/molxK	1302.53	Joback Method
cpg	1803.86	J/molxK	1346.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392803&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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