

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

InChI: InChI=1S/C32H61NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-36-31(34)28(5)
InChIKey: FGHXSSIIIXJENQB-UHFFFAOYSA-N

Formula: C32H61NO4

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

Mol. weight [g/mol]: 523.83

Physical Properties

Property code	Value	Unit	Source
gf	-134.35	kJ/mol	Joback Method
hf	-1122.80	kJ/mol	Joback Method
hfus	74.16	kJ/mol	Joback Method
hvap	106.22	kJ/mol	Joback Method
log10ws	-9.88		Crippen Method
logp	9.319		Crippen Method
mvol	475.740	ml/mol	McGowan Method
pc	611.17	kPa	Joback Method
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
tb	1105.91	K	Joback Method
tc	1382.73	K	Joback Method
tf	596.09	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1784.16	J/molxK	1105.91	Joback Method
cpg	1805.35	J/molxK	1152.05	Joback Method
cpg	1823.35	J/molxK	1198.18	Joback Method
cpg	1838.31	J/molxK	1244.32	Joback Method
cpg	1850.37	J/molxK	1290.46	Joback Method
cpg	1859.65	J/molxK	1336.59	Joback Method
cpg	1866.31	J/molxK	1382.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392804&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
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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