

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

Inchi: InChI=1S/C33H63NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-37-32(35)
InchiKey: NGPGFZRECDSDNR-UHFFFAOYSA-N

Formula: C33H63NO4

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

Mol. weight [g/mol]: 537.86

Physical Properties

Property code	Value	Unit	Source
gf	-125.93	kJ/mol	Joback Method
hf	-1143.44	kJ/mol	Joback Method
hfus	76.75	kJ/mol	Joback Method
hvap	108.44	kJ/mol	Joback Method
log10ws	-10.30		Crippen Method
logp	9.709		Crippen Method
mcvol	489.830	ml/mol	McGowan Method
pc	583.16	kPa	Joback Method
rinpol	3462.00		NIST Webbook
rinpol	3462.00		NIST Webbook
tb	1128.79	K	Joback Method
tc	1420.73	K	Joback Method
tf	607.36	K	Joback Method
vc	1.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1849.20	J/molxK	1128.79	Joback Method
cpg	1870.60	J/molxK	1177.45	Joback Method
cpg	1888.48	J/molxK	1226.10	Joback Method
cpg	1903.02	J/molxK	1274.76	Joback Method
cpg	1914.39	J/molxK	1323.41	Joback Method
cpg	1922.76	J/molxK	1372.07	Joback Method
cpg	1928.29	J/molxK	1420.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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