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

Inchi: InChI=1S/C23H43NO4/c1-7-8-9-10-11-12-15-27-22(25)19(5)24(6)23(26)28-21-16-18(4)1
InchiKey: DECALBIKVGJZIN-UHFFFAOYSA-N
Formula: C23H43NO4
SMILES: CCCCCCCCOC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
gf	-210.13	kJ/mol	Joback Method
hf	-937.04	kJ/mol	Joback Method
hfus	50.85	kJ/mol	Joback Method
hvap	86.18	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.808		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
pc	988.26	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	899.99	K	Joback Method
tc	1103.97	K	Joback Method
tf	494.66	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.47	J/mol×K	899.99	Joback Method
cpg	1224.40	J/mol×K	933.99	Joback Method
cpg	1242.70	J/mol×K	967.98	Joback Method
cpg	1259.39	J/mol×K	1001.98	Joback Method
cpg	1274.49	J/mol×K	1035.98	Joback Method
cpg	1288.05	J/mol×K	1069.97	Joback Method
cpg	1300.09	J/mol×K	1103.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392796&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
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
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