1-Aminocyclopentanecarboxylic acid, N-((1R)-(-)-menthyloxycarbonyl)-, dodecyl ester

Inchi: InChI=1S/C29H53NO4/c1-5-6-7-8-9-10-11-12-13-16-21-33-27(31)29(19-14-15-20-29)30-
InchiKey: AEUBGSANOZQKRL-UHFFFAOYSA-N
Formula: C29H53NO4
SMILES: CCCCCCCCCCCCOC(=O)C1(NC(=O)OC2CC(C)CCC2C(C)C)CCCC1
Mol. weight [g/mol]: 479.74

Physical Properties

Property code	Value	Unit	Source
gf	-147.50	kJ/mol	Joback Method
hf	-993.94	kJ/mol	Joback Method
hfus	59.63	kJ/mol	Joback Method
hvap	103.42	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	7.950		Crippen Method
mcvol	422.610	ml/mol	McGowan Method
pc	804.79	kPa	Joback Method
rinpol	3132.00		NIST Webbook
rinpol	3132.00		NIST Webbook
tb	1090.96	K	Joback Method
tc	1339.44	K	Joback Method
tf	632.27	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1618.98	J/mol×K	1090.96	Joback Method
cpg	1645.35	J/mol×K	1132.37	Joback Method
cpg	1670.84	J/mol×K	1173.79	Joback Method
cpg	1695.68	J/mol×K	1215.20	Joback Method
cpg	1720.08	J/mol×K	1256.61	Joback Method
cpg	1744.25	J/mol×K	1298.02	Joback Method
cpg	1768.41	J/mol×K	1339.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392619&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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