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

Inchi: InChI=1S/C27H49NO4/c1-5-6-7-8-9-10-11-14-19-31-25(29)27(17-12-13-18-27)28-26(30)

InchiKey: GNJKKYVXOLBUPV-UHFFFAOYSA-N

Formula: C27H49NO4

SMILES: CCCCCCCCCCOC(=O)C1(N=C(O)OC2CC(C)CCC2C(C)C)CCCC1

Mol. weight [g/mol]: 451.68

Physical Properties

Property code	Value	Unit	Source
hf	-973.35	kJ/mol	Joback Method
hvap	105.86	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.375		Crippen Method
mcvol	394.430	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	2924.00		NIST Webbook
rinpol	2924.00		NIST Webbook
tb	1109.90	K	Joback Method
tc	1363.72	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392617&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

hf: Enthalpy of formation 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

Latest version available from:
https://www.chemeo.com/cid/94-825-2/1-Aminocyclopentanecarboxylic-acid-N-1R-menthyloxycarbonyl-decyl-ester.p
Generated by Cheméo on 2024-04-23 15:55:52.073444871 +0000 UTC m=+16177000.994022199.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.