1-Aminocyclopentanecarboxylic acid, N-(neopentyloxycarbonyl)-, tridecyl ester

Inchi: InChI=1S/C25H47NO4/c1-5-6-7-8-9-10-11-12-13-14-17-20-29-22(27)25(18-15-16-19-25)

InchiKey: NFQSKHZZJRJBAG-UHFFFAOYSA-N

Formula: C25H47NO4

SMILES: CCCCCCCCCCCCCOC(=O)C1(N=C(O)OCC(C)(C)C)CCCC1

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
hf	-949.18	kJ/mol	Joback Method
hvap	100.69	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.130		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
pc	889.47	kPa	Joback Method
rinpol	2845.00		NIST Webbook
tb	1051.14	K	Joback Method
tc	1291.40	K	Joback Method

Sources

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=U392523&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/95-439-0/1-Aminocyclopentanecarboxylic-acid-N-neopentyloxycarbonyl-tridecyl-ester.p

Generated by Cheméo on 2024-10-12 09:11:03.095137543 +0000 UTC m=+3305125.732106791.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.