

1-Aminocyclopentanecarboxylic acid, N-(neopentylloxycarbonyl)-, 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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392523&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

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

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