1-Aminocyclopentanecarboxylic acid, N-(propoxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C15H27NO4/c1-3-5-8-12-19-13(17)15(9-6-7-10-15)16-14(18)20-11-4-2/h3-12H

InchiKey: CPDSDLRYZMJWJQ-UHFFFAOYSA-N

Formula: C15H27NO4

SMILES: CCCCCOC(=O)C1(N=C(O)OCCC)CCCC1

Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
hf	-734.03	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.373		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	825.57	K	Joback Method
tc	1027.01	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=U392489&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