1-Aminocyclopentanecarboxylic acid, N-hexyloxycarbonyl-, heptyl ester

Inchi: InChI=1S/C20H37NO4/c1-3-5-7-9-13-16-24-18(22)20(14-10-11-15-20)21-19(23)25-17-12

InchiKey: OPUSZINVBJDFFH-UHFFFAOYSA-N

Formula: C20H37NO4

SMILES: CCCCCCCOC(=O)C1(N=C(O)OCCCCCC)CCCC1

Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
hf	-837.23	kJ/mol	Joback Method
hvap	90.86	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.324		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	939.97	K	Joback Method
tc	1151.31	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=U392429&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

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