2-Aminopent-4-enoic acid, N-(2-benzyloxyetoxycarbonyl)-, heptyl ester

Inchi: InChI=1S/C22H33NO5/c1-3-5-6-7-11-15-27-21(24)20(12-4-2)23-22(25)28-17-16-26-18-1
InchiKey: NNQJTEVGCHJBDO-UHFFFAOYSA-N
Formula: C22H33NO5
SMILES: C=CCC(N=C(O)OCCOCc1ccccc1)C(=O)OCCCCCCC
Mol. weight [g/mol]: 391.50

Physical Properties

Property code	Value	Unit	Source
hf	-729.77	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.592		Crippen Method
mcvol	323.510	ml/mol	McGowan Method
pc	1153.00	kPa	Joback Method
rinpol	2893.00		NIST Webbook
rinpol	2893.00		NIST Webbook
tb	1015.55	K	Joback Method
tc	1243.72	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393184&Units=SI

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