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

Inchi: InChI=1S/C21H31NO5/c1-3-5-6-10-14-26-20(23)19(11-4-2)22-21(24)27-16-15-25-17-18-

InchiKey: GIFGUSFWVZZUEE-UHFFFAOYSA-N

Formula: C21H31NO5

SMILES: C=CCC(N=C(O)OCCOCc1ccccc1)C(=O)OCCCCCC

Mol. weight [g/mol]: 377.47

Physical Properties

Property code	Value	Unit	Source
hf	-709.13	kJ/mol	Joback Method
hvap	97.61	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.202		Crippen Method
mcvol	309.420	ml/mol	McGowan Method
pc	1232.01	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	992.67	K	Joback Method
tc	1215.32	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=U393183&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