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

Inchi: InChI=1S/C19H27NO5/c1-4-8-17(18(21)25-13-15(2)3)20-19(22)24-12-11-23-14-16-9-6-5

InchiKey: DOBAJINZPKDZFK-UHFFFAOYSA-N

Formula: C19H27NO5

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

Mol. weight [g/mol]: 349.42

Physical Properties

Property code	Value	Unit	Source
hf	-673.13	kJ/mol	Joback Method
hvap	92.77	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.278		Crippen Method
mcvol	281.240	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook
tb	946.47	K	Joback Method
tc	1162.00	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393181&Units=SI

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

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