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

Inchi: InChI=1S/C19H27NO5/c1-3-5-12-24-18(21)17(9-4-2)20-19(22)25-14-13-23-15-16-10-7-6

InchiKey: DPMNDWRQUQEEKW-UHFFFAOYSA-N

Formula: C19H27NO5

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

Mol. weight [g/mol]: 349.42

Physical Properties

Property code	Value	Unit	Source
hf	-667.85	kJ/mol	Joback Method
hvap	93.16	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.422		Crippen Method
mcvol	281.240	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	946.91	K	Joback Method
tc	1161.62	K	Joback Method

Sources

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=U393182&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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