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

Inchi: InChI=1S/C24H37NO5/c1-3-5-6-7-8-9-13-17-29-23(26)22(14-4-2)25-24(27)30-19-18-28-
InchiKey: AKWCQIUGEOJNSW-UHFFFAOYSA-N
Formula: C24H37NO5
SMILES: C=CCC(N=C(O)OCCOCc1ccccc1)C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 419.55

Physical Properties

Property code	Value	Unit	Source
hf	-771.05	kJ/mol	Joback Method
hvap	104.28	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.372		Crippen Method
mcvol	351.690	ml/mol	McGowan Method
pc	1016.18	kPa	Joback Method
rinpol	2998.00		NIST Webbook
rinpol	2998.00		NIST Webbook
tb	1061.31	K	Joback Method
tc	1304.00	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393186&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