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

Inchi: InChI=1S/C25H39NO5/c1-3-5-6-7-8-9-10-14-18-30-24(27)23(15-4-2)26-25(28)31-20-19-
InchiKey: VMFOJBNCIYEODN-UHFFFAOYSA-N
Formula: C25H39NO5
SMILES: C=CCC(N=C(O)OCCOCc1ccccc1)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 433.58

Physical Properties

Property code	Value	Unit	Source
hf	-791.69	kJ/mol	Joback Method
hvap	106.51	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.762		Crippen Method
mcvol	365.780	ml/mol	McGowan Method
pc	956.73	kPa	Joback Method
rinpol	3100.00		NIST Webbook
rinpol	3100.00		NIST Webbook
tb	1084.19	K	Joback Method
tc	1336.05	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=U393187&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