2-Aminopent-4-enoic acid, N-hexyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C23H43NO4/c1-4-7-9-11-12-13-14-15-17-19-27-22(25)21(18-6-3)24-23(26)28-

InchiKey: XUXDJWHJFMDIKA-UHFFFAOYSA-N

Formula: C23H43NO4

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

Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
hf	-854.72	kJ/mol	Joback Method
hvap	97.37	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.516		Crippen Method
mcvol	355.490	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	989.33	K	Joback Method
tc	1218.87	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=U393144&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