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

Inchi: InChI=1S/C21H39NO4/c1-4-7-9-11-12-13-15-17-25-20(23)19(16-6-3)22-21(24)26-18-14-

InchiKey: UMIBHDQQBHAXFG-UHFFFAOYSA-N

Formula: C21H39NO4

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

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
hf	-813.44	kJ/mol	Joback Method
hvap	92.92	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.736		Crippen Method
mcvol	327.310	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	943.57	K	Joback Method
tc	1156.81	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=U393142&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