2-Aminopent-4-enoic acid, N-octyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C22H41NO4/c1-4-7-9-11-13-15-18-26-21(24)20(17-6-3)23-22(25)27-19-16-14-

InchiKey: CMCGVYXSNLJGTO-UHFFFAOYSA-N

Formula: C22H41NO4

SMILES: C=CCC(N=C(O)OCCCCCCCC)C(=O)OCCCCCCCC

Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
hf	-834.08	kJ/mol	Joback Method
hvap	95.15	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	6.126		Crippen Method
mcvol	341.400	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	966.45	K	Joback Method
tc	1187.24	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=U393154&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