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

Inchi: InChI=1S/C24H45NO4/c1-4-7-9-11-13-14-16-18-21-29-24(27)25-22(19-6-3)23(26)28-20-

InchiKey: GXCAIZSRJGQPJM-UHFFFAOYSA-N

Formula: C24H45NO4

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

Mol. weight [g/mol]: 411.62

Physical Properties

Property code	Value	Unit	Source
hf	-875.36	kJ/mol	Joback Method
hvap	99.60	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.906		Crippen Method
mcvol	369.580	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinpol	2737.00		NIST Webbook
rinpol	2737.00		NIST Webbook
tb	1012.21	K	Joback Method
tc	1251.78	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393174&Units=SI

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