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

Inchi: InChI=1S/C17H31NO4/c1-4-7-9-11-14-22-17(20)18-15(12-6-3)16(19)21-13-10-8-5-2/h6,1

InchiKey: OPPAHBLNEHQMSM-UHFFFAOYSA-N

Formula: C17H31NO4

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

Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
hf	-730.88	kJ/mol	Joback Method
hvap	84.02	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.175		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	852.05	K	Joback Method
tc	1045.38	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393140&Units=SI

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

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

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