2-Aminopent-4-enoic acid, N-(2-ethylhexyloxycarbonyl)-, isobutyl ester

Inchi: InChI=1S/C18H33NO4/c1-6-9-11-15(8-3)13-23-18(21)19-16(10-7-2)17(20)22-12-14(4)5/h

InchiKey: KBNVZJYEUURFJI-UHFFFAOYSA-N

Formula: C18H33NO4

SMILES: C=CCC(N=C(O)OCC(CC)CCCC)C(=O)OCC(C)C

Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
hf	-762.08	kJ/mol	Joback Method
hvap	85.47	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.277		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	874.05	K	Joback Method
tc	1071.93	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393160&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

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