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

Inchi: InChI=1S/C20H37NO4/c1-5-9-11-12-15-24-19(22)18(13-7-3)21-20(23)25-16-17(8-4)14-1

InchiKey: FMKQOURDRHXBOQ-UHFFFAOYSA-N

Formula: C20H37NO4

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

Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
hf	-798.08	kJ/mol	Joback Method
hvap	90.31	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.202		Crippen Method
mcvol	313.220	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	2269.00		NIST Webbook
rinpol	2269.00		NIST Webbook
tb	920.25	K	Joback Method
tc	1126.72	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=U393162&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