

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

Inchi: InChI=1S/C27H51NO4/c1-4-7-9-11-13-14-15-16-17-19-20-23-31-26(29)25(22-6-3)28-27
InchiKey: KNHLOWWHLJPXTK-UHFFFAOYSA-N
Formula: C27H51NO4
SMILES: C=CCC(N=C(O)OCCCCCCCC)C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
hf	-937.28	kJ/mol	Joback Method
hvap	106.28	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	8.076		Crippen Method
mcvol	411.850	ml/mol	McGowan Method
pc	715.30	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	1080.85	K	Joback Method
tc	1359.32	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U393159&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

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