

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

Inchi:	InChI=1S/C28H53NO4/c1-4-7-9-11-13-15-16-18-19-21-24-32-27(30)26(23-6-3)29-28(31)
InchiKey:	RDLLLIWWKBURFO-UHFFFAOYSA-N
Formula:	C28H53NO4
SMILES:	C=CCC(N=C(O)OCCCCCCCCC)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]:	467.72

Physical Properties

Property code	Value	Unit	Source
hf	-957.92	kJ/mol	Joback Method
hvap	108.50	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	8.466		Crippen Method
mcvol	425.940	ml/mol	McGowan Method
pc	679.94	kPa	Joback Method
rinpol	3136.00		NIST Webbook
rinpol	3136.00		NIST Webbook
tb	1103.73	K	Joback Method
tc	1398.51	K	Joback Method

Sources

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=U393178&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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