

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

Inchi:	InChI=1S/C23H43NO4/c1-4-7-9-11-13-15-16-19-27-22(25)21(18-6-3)24-23(26)28-20-17
InchiKey:	CYDFTXIVMSCYPD-UHFFFAOYSA-N
Formula:	C23H43NO4
SMILES:	<chem>C=CCC(N=C(O)OCCCCCCCC)C(=O)OCCCCCCCC</chem>
Mol. weight [g/mol]:	397.59

Physical Properties

Property code	Value	Unit	Source
hf	-854.72	kJ/mol	Joback Method
hvap	97.37	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.516		Crippen Method
mcvol	355.490	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	989.33	K	Joback Method
tc	1218.87	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=U393155&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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