

L-Norvaline, n-propoxycarbonyl-, octadecyl ester

Inchi:	InChI=1S/C27H53NO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-31-26(29)2
InchiKey:	ZLJCCRORTBHPBD-UHFFFAOYSA-N
Formula:	C27H53NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CCC)N=C(O)OCCC
Mol. weight [g/mol]:	455.71

Physical Properties

Property code	Value	Unit	Source
hf	-1062.71	kJ/mol	Joback Method
hvap	106.95	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	8.300		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	699.50	kPa	Joback Method
tb	1084.17	K	Joback Method
tc	1368.09	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=U320743&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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