

L-Norvaline, N-hexyloxycarbonyl-, tridecyl ester

Inchi:	InChI=1S/C25H49NO4/c1-4-7-9-11-12-13-14-15-16-17-19-21-29-24(27)23(20-6-3)26-25
InchiKey:	VYMDAGQQDAYLQZ-HSZRJFAPSA-N
Formula:	C25H49NO4
SMILES:	CCCCCCCCCCCCCOC(=O)C(CCC)N=C(O)OCCCCC
Mol. weight [g/mol]:	427.66

Physical Properties

Property code	Value	Unit	Source
hf	-1021.43	kJ/mol	Joback Method
hvap	102.49	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.520		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	776.34	kPa	Joback Method
rinpol	2889.00		NIST Webbook
rinpol	2889.00		NIST Webbook
tb	1038.41	K	Joback Method
tc	1293.43	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=U392839&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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