D-Alanine, N-neopentyloxycarbonyl-, nonyl ester

Inchi: InChI=1S/C18H35NO4/c1-6-7-8-9-10-11-12-13-22-16(20)15(2)19-17(21)23-14-18(3,4)5/h

InchiKey: ZTIORUIPMXZEFV-UHFFFAOYSA-N

Formula: C18H35NO4

SMILES: CCCCCCCCCOC(=O)C(C)N=C(O)OCC(C)(C)C

Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
hf	-885.70	kJ/mol	Joback Method
hvap	85.62	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.645		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1190.70	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	875.02	K	Joback Method
tc	1072.96	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U347767&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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