D-Alanine, N-neopentyloxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C24H47NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-28-22(26)21(2)25-23(

InchiKey: ZWVVXVIBCRAKBN-UHFFFAOYSA-N

Formula: C24H47NO4

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

Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
hf	-1009.54	kJ/mol	Joback Method
hvap	98.97	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.986		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	828.59	kPa	Joback Method
rinpol	2703.00		NIST Webbook
rinpol	2703.00		NIST Webbook
tb	1012.30	K	Joback Method
tc	1248.52	K	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U347773&Units=SI

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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