D-Alanine, N-neopentyloxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C21H41NO4/c1-6-7-8-9-10-11-12-13-14-15-16-25-19(23)18(2)22-20(24)26-17-

InchiKey: OXSDEGJPWDHGBP-UHFFFAOYSA-N

Formula: C21H41NO4

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

Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
hf	-947.62	kJ/mol	Joback Method
hvap	92.29	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.816		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	985.16	kPa	Joback Method
rinpol	2406.00		NIST Webbook
rinpol	2406.00		NIST Webbook
tb	943.66	K	Joback Method
tc	1155.92	K	Joback Method

Sources

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=U347770&Units=SI

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

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

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