D-Alanine, N-neopentyloxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C26H51NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-30-24(28)23(2)
InchiKey: JLCGGTGMMPIEOA-UHFFFAOYSA-N
Formula: C26H51NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)N=C(O)OCC(C)(C)C
Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
hf	-1050.82	kJ/mol	Joback Method
hvap	103.42	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.766		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	744.07	kPa	Joback Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tb	1058.06	K	Joback Method
tc	1316.79	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=U347775&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