L-Norvaline, N-allyloxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C21H39NO4/c1-4-7-8-9-10-11-12-13-14-15-18-25-20(23)19(16-5-2)22-21(24)2

InchiKey: QHYUSWUIKRYFFW-UHFFFAOYSA-N

Formula: C21H39NO4

SMILES: C=CCOC(=O)NC(CCC)C(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 369.55

Physical Properties

Property code	Value	Unit	Source
hfus	56.02	kJ/mol	Joback Method
log10ws	-5.65		Cheméo Relay (1.0)
logp	5.531		Crippen Method
mcvol	327.310	ml/mol	McGowan Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	636.05	K	Cheméo Relay (1.0)
tf	301.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.24	J/mol×K	878.87	Joback Method
cpg	1084.96	J/mol×K	911.74	Joback Method
cpg	1101.49	J/mol×K	944.62	Joback Method
cpg	1116.84	J/mol×K	977.49	Joback Method
cpg	1131.05	J/mol×K	1010.37	Joback Method
cpg	1144.16	J/mol×K	1043.24	Joback Method
cpg	1156.18	J/mol×K	1076.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320752&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point