L-Norvaline, N-allyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C17H31NO4/c1-4-7-8-9-10-11-14-21-16(19)15(12-5-2)18-17(20)22-13-6-3/h6,1
InchiKey: WPOZNBKUDJCGDA-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: C=CCOC(=O)NC(CCC)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 313.44

Physical Properties

Property code	Value	Unit	Source
hfus	45.66	kJ/mol	Joback Method
log10ws	-4.40		Cheméo Relay (1.0)
logp	3.971		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	605.41	K	Cheméo Relay (1.0)
tf	282.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.43	J/mol×K	787.35	Joback Method
cpg	843.61	J/mol×K	818.24	Joback Method
cpg	858.86	J/mol×K	849.12	Joback Method
cpg	873.18	J/mol×K	880.01	Joback Method
cpg	886.59	J/mol×K	910.89	Joback Method
cpg	899.10	J/mol×K	941.78	Joback Method
cpg	910.75	J/mol×K	972.66	Joback Method

Sources

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320748&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

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

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