L-Norvaline, N-allyoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-30-25(28)24(21
InchiKey: VLJGJTNRUSFHBO-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: C=CCOC(=O)NC(CCC)C(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 439.68

Physical Properties

Property code	Value	Unit	Source
hfus	68.97	kJ/mol	Joback Method
log10ws	-7.22		Cheméo Relay (1.0)
logp	7.482		Crippen Method
mcvol	397.760	ml/mol	McGowan Method
tb	670.25	K	Cheméo Relay (1.0)
tf	318.05	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.02	J/mol×K	993.27	Joback Method
cpg	1401.26	J/mol×K	1032.19	Joback Method
cpg	1419.70	J/mol×K	1071.10	Joback Method
cpg	1436.42	J/mol×K	1110.02	Joback Method
cpg	1451.48	J/mol×K	1148.93	Joback Method
cpg	1464.95	J/mol×K	1187.85	Joback Method
cpg	1476.91	J/mol×K	1226.77	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=U320756&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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point