l-Norvaline, N-allyloxycarbonyl-, allyl ester

Inchi: InChI=1S/C12H19NO4/c1-4-7-10(11(14)16-8-5-2)13-12(15)17-9-6-3/h5-6,10H,2-4,7-9H2
InchiKey: AARSMYVFHVHAGU-UHFFFAOYSA-N
Formula: C12H19NO4
SMILES: C=CCOC(=O)NC(CCC)C(=O)OCC=C
Mol. weight [g/mol]: 241.28

Physical Properties

Property code	Value	Unit	Source
gf	-155.05	kJ/mol	Joback Method
hf	-481.56	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	65.33	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	1.796		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1537.00		NIST Webbook
tb	669.63	K	Joback Method
tc	857.27	K	Joback Method
tf	403.46	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.95	J/mol×K	669.63	Joback Method
cpg	539.45	J/mol×K	700.90	Joback Method
cpg	552.24	J/mol×K	732.18	Joback Method
cpg	564.33	J/mol×K	763.45	Joback Method
cpg	575.72	J/mol×K	794.72	Joback Method
cpg	586.43	J/mol×K	825.99	Joback Method
cpg	596.45	J/mol×K	857.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320758&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume