l-Norvaine, N-allyloxycarbonyl-, decyl ester

Inchi: InChI=1S/C19H35NO4/c1-4-7-8-9-10-11-12-13-16-23-18(21)17(14-5-2)20-19(22)24-15-6
InchiKey: AVIUNEKVERFNIN-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: C=CCOC(=O)NC(CCC)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
gf	-183.95	kJ/mol	Joback Method
hf	-751.47	kJ/mol	Joback Method
hfus	50.84	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.751		Crippen Method
mcvol	299.130	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	833.11	K	Joback Method
tc	1022.82	K	Joback Method
tf	484.11	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.79	J/mol×K	833.11	Joback Method
cpg	962.72	J/mol×K	864.73	Joback Method
cpg	978.60	J/mol×K	896.35	Joback Method
cpg	993.44	J/mol×K	927.97	Joback Method
cpg	1007.27	J/mol×K	959.58	Joback Method
cpg	1020.11	J/mol×K	991.20	Joback Method
cpg	1031.99	J/mol×K	1022.82	Joback Method

Sources

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=U320751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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