«beta»-Alanine, N-allyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C18H33NO4/c1-3-5-6-7-8-9-10-11-12-16-22-17(20)13-14-19-18(21)23-15-4-2/h
InchiKey: PGGHNNHJJKVVET-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: C=CCOC(=O)NCCC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
gf	-189.93	kJ/mol	Joback Method
hf	-725.55	kJ/mol	Joback Method
hfus	51.77	kJ/mol	Joback Method
hvap	79.74	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.363		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	810.67	K	Joback Method
tc	996.79	K	Joback Method
tf	487.84	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.68	J/mol×K	810.67	Joback Method
cpg	902.15	J/mol×K	841.69	Joback Method
cpg	917.64	J/mol×K	872.71	Joback Method
cpg	932.17	J/mol×K	903.73	Joback Method
cpg	945.77	J/mol×K	934.75	Joback Method
cpg	958.44	J/mol×K	965.77	Joback Method
cpg	970.22	J/mol×K	996.79	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=U321039&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