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

Inchi: InChI=1S/C14H25NO4/c1-3-5-6-7-8-12-18-13(16)9-10-15-14(17)19-11-4-2/h4H,2-3,5-12

InchiKey: RCTAKIGNHOORQU-UHFFFAOYSA-N

Formula: C14H25NO4

SMILES: C=CCOC(=O)NCCC(=O)OCCCCCCC

Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
gf	-223.61	kJ/mol	Joback Method
hf	-642.99	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	70.84	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.802		Crippen Method
mcvol	228.680	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1955.00		NIST Webbook
tb	719.15	K	Joback Method
tc	900.53	K	Joback Method
tf	442.76	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.43	J/mol×K	719.15	Joback Method
cpg	671.24	J/mol×K	749.38	Joback Method
cpg	685.28	J/mol×K	779.61	Joback Method
cpg	698.55	J/mol×K	809.84	Joback Method
cpg	711.07	J/mol×K	840.07	Joback Method
cpg	722.83	J/mol×K	870.30	Joback Method
cpg	733.85	J/mol×K	900.53	Joback Method

Sources

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=U321035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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