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

Inchi: InChI=1S/C13H23NO4/c1-3-5-6-7-11-17-12(15)8-9-14-13(16)18-10-4-2/h4H,2-3,5-11H2,

InchiKey: XINYMSULHNNZRJ-UHFFFAOYSA-N

Formula: C13H23NO4

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

Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
gf	-232.03	kJ/mol	Joback Method
hf	-622.35	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	68.61	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.412		Crippen Method
mcvol	214.590	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	696.27	K	Joback Method
tc	877.89	K	Joback Method
tf	431.49	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.82	J/mol×K	696.27	Joback Method
cpg	616.16	J/mol×K	726.54	Joback Method
cpg	629.78	J/mol×K	756.81	Joback Method
cpg	642.67	J/mol×K	787.08	Joback Method
cpg	654.84	J/mol×K	817.35	Joback Method
cpg	666.29	J/mol×K	847.62	Joback Method
cpg	677.05	J/mol×K	877.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321034&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