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

Inchi: InChI=1S/C21H39NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-19-25-20(23)16-17-22-21(24)2

InchiKey: GSWSKDQNNCXWKF-UHFFFAOYSA-N

Formula: C21H39NO4

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

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
gf	-164.67	kJ/mol	Joback Method
hf	-787.47	kJ/mol	Joback Method
hfus	59.54	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.533		Crippen Method
mcvol	327.310	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2667.00		NIST Webbook
tb	879.31	K	Joback Method
tc	1076.53	K	Joback Method
tf	521.65	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.77	J/mol×K	879.31	Joback Method
cpg	1084.51	J/mol×K	912.18	Joback Method
cpg	1101.06	J/mol×K	945.05	Joback Method
cpg	1116.45	J/mol×K	977.92	Joback Method
cpg	1130.71	J/mol×K	1010.79	Joback Method
cpg	1143.87	J/mol×K	1043.66	Joback Method
cpg	1155.96	J/mol×K	1076.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321041&Units=SI

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

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