«beta»-Alanine, N-(3-methylbut-2-enoyl)-, tetradecyl ester

Inchi: InChI=1S/C22H41NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-26-22(25)16-17-23-21(24)1

InchiKey: RRRWSPCXSJBNIK-UHFFFAOYSA-N

Formula: C22H41NO3

SMILES: CCCCCCCCCCCCCCOC(=O)CCNC(=O)C=C(C)C

Mol. weight [g/mol]: 367.57

Physical Properties

Property code	Value	Unit	Source
gf	-67.42	kJ/mol	Joback Method
hf	-693.89	kJ/mol	Joback Method
hfus	61.11	kJ/mol	Joback Method
hvap	86.94	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.703		Crippen Method
mcvol	335.530	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		NIST Webbook
tb	887.13	K	Joback Method
tc	1086.22	K	Joback Method
tf	493.41	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.45	J/mol×K	887.13	Joback Method
cpg	1116.94	J/mol×K	920.31	Joback Method
cpg	1134.32	J/mol×K	953.49	Joback Method
cpg	1150.64	J/mol×K	986.68	Joback Method
cpg	1165.95	J/mol×K	1019.86	Joback Method
cpg	1180.32	J/mol×K	1053.04	Joback Method
cpg	1193.78	J/mol×K	1086.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321956&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

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