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

Inchi: InChI=1S/C24H45NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-28-24(27)18-19-25-2

InchiKey: QKRGLEQGMQJVGW-UHFFFAOYSA-N

Formula: C24H45NO3

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

Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
gf	-50.58	kJ/mol	Joback Method
hf	-735.17	kJ/mol	Joback Method
hfus	66.29	kJ/mol	Joback Method
hvap	91.39	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.483		Crippen Method
mcvol	363.710	ml/mol	McGowan Method
pc	894.80	kPa	Joback Method
rinpol	3108.00		NIST Webbook
tb	932.89	K	Joback Method
tc	1143.22	K	Joback Method
tf	515.95	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.72	J/mol×K	932.89	Joback Method
cpg	1243.29	J/mol×K	967.94	Joback Method
cpg	1261.61	J/mol×K	1003.00	Joback Method
cpg	1278.74	J/mol×K	1038.05	Joback Method
cpg	1294.75	J/mol×K	1073.11	Joback Method
cpg	1309.72	J/mol×K	1108.16	Joback Method
cpg	1323.70	J/mol×K	1143.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321958&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