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

Inchi: InChI=1S/C23H43NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-27-23(26)17-18-24-22(2

InchiKey: KQNFLSLDFIYHLY-UHFFFAOYSA-N

Formula: C23H43NO3

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

Mol. weight [g/mol]: 381.59

Physical Properties

Property code	Value	Unit	Source
gf	-59.00	kJ/mol	Joback Method
hf	-714.53	kJ/mol	Joback Method
hfus	63.70	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.093		Crippen Method
mcvol	349.620	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	2944.00		NIST Webbook
tb	910.01	K	Joback Method
tc	1114.22	K	Joback Method
tf	504.68	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.78	J/mol×K	910.01	Joback Method
cpg	1179.78	J/mol×K	944.05	Joback Method
cpg	1197.61	J/mol×K	978.08	Joback Method
cpg	1214.32	J/mol×K	1012.12	Joback Method
cpg	1229.97	J/mol×K	1046.15	Joback Method
cpg	1244.63	J/mol×K	1080.19	Joback Method
cpg	1258.34	J/mol×K	1114.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321957&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