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

Inchi: InChI=1S/C15H27NO3/c1-4-5-6-7-8-11-19-15(18)9-10-16-14(17)12-13(2)3/h12H,4-11H2

InchiKey: LIIAZXYMSXEAJJ-UHFFFAOYSA-N

Formula: C15H27NO3

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

Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
gf	-126.36	kJ/mol	Joback Method
hf	-549.41	kJ/mol	Joback Method
hfus	42.98	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.972		Crippen Method
mcvol	236.900	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2084.00		NIST Webbook
tb	726.97	K	Joback Method
tc	912.58	K	Joback Method
tf	414.52	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.12	J/mol×K	726.97	Joback Method
cpg	699.73	J/mol×K	757.90	Joback Method
cpg	714.52	J/mol×K	788.84	Joback Method
cpg	728.52	J/mol×K	819.77	Joback Method
cpg	741.76	J/mol×K	850.71	Joback Method
cpg	754.26	J/mol×K	881.64	Joback Method
cpg	766.05	J/mol×K	912.58	Joback Method

Sources

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=U321953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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