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

Inchi: InChI=1S/C16H29NO3/c1-4-5-6-7-8-9-12-20-16(19)10-11-17-15(18)13-14(2)3/h13H,4-12

InchiKey: RJGHMGYFMHNHKK-UHFFFAOYSA-N

Formula: C16H29NO3

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

Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
gf	-117.94	kJ/mol	Joback Method
hf	-570.05	kJ/mol	Joback Method
hfus	45.57	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.363		Crippen Method
mcvol	250.990	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2178.00		NIST Webbook
tb	749.85	K	Joback Method
tc	935.41	K	Joback Method
tf	425.79	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.50	J/mol×K	749.85	Joback Method
cpg	756.51	J/mol×K	780.78	Joback Method
cpg	771.67	J/mol×K	811.70	Joback Method
cpg	786.01	J/mol×K	842.63	Joback Method
cpg	799.56	J/mol×K	873.56	Joback Method
cpg	812.35	J/mol×K	904.48	Joback Method
cpg	824.41	J/mol×K	935.41	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=U321954&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