L-Valine, N-(3-methylbut-2-enoyl)-, hexyl ester

Inchi: InChI=1S/C16H29NO3/c1-6-7-8-9-10-20-16(19)15(13(4)5)17-14(18)11-12(2)3/h11,13,15
InchiKey: KQVAHKLHMYTIKP-UHFFFAOYSA-N
Formula: C16H29NO3
SMILES: CCCCCCOC(=O)C(NC(=O)C=C(C)C)C(C)C
Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
gf	-122.82	kJ/mol	Joback Method
hf	-580.61	kJ/mol	Joback Method
hfus	38.53	kJ/mol	Joback Method
hvap	72.81	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.217		Crippen Method
mcvol	250.990	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	748.97	K	Joback Method
tc	938.77	K	Joback Method
tf	395.79	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.53	J/mol×K	748.97	Joback Method
cpg	757.93	J/mol×K	780.60	Joback Method
cpg	773.42	J/mol×K	812.24	Joback Method
cpg	788.04	J/mol×K	843.87	Joback Method
cpg	801.82	J/mol×K	875.51	Joback Method
cpg	814.78	J/mol×K	907.14	Joback Method
cpg	826.96	J/mol×K	938.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346070&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