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

Inchi: InChI=1S/C17H31NO3/c1-6-7-8-9-10-11-21-17(20)16(14(4)5)18-15(19)12-13(2)3/h12,14
InchiKey: OXCDCQWYQJSHMV-UHFFFAOYSA-N
Formula: C17H31NO3
SMILES: CCCCCCCOC(=O)C(NC(=O)C=C(C)C)C(C)C
Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
gf	-114.40	kJ/mol	Joback Method
hf	-601.25	kJ/mol	Joback Method
hfus	41.12	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.607		Crippen Method
mcvol	265.080	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
tb	771.85	K	Joback Method
tc	961.60	K	Joback Method
tf	407.06	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.96	J/mol×K	771.85	Joback Method
cpg	815.69	J/mol×K	803.48	Joback Method
cpg	831.49	J/mol×K	835.10	Joback Method
cpg	846.39	J/mol×K	866.73	Joback Method
cpg	860.42	J/mol×K	898.35	Joback Method
cpg	873.61	J/mol×K	929.98	Joback Method
cpg	886.01	J/mol×K	961.60	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=U346071&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

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