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

Inchi: InChI=1S/C13H23NO3/c1-6-7-17-13(16)12(10(4)5)14-11(15)8-9(2)3/h8,10,12H,6-7H2,1-

InchiKey: QOVHIZMKMNZFNV-UHFFFAOYSA-N

Formula: C13H23NO3

SMILES: CCCOC(=O)C(NC(=O)C=C(C)C)C(C)C

Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
gf	-148.08	kJ/mol	Joback Method
hf	-518.69	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.047		Crippen Method
mcvol	208.720	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	680.33	K	Joback Method
tc	873.36	K	Joback Method
tf	361.98	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.80	J/mol×K	680.33	Joback Method
cpg	591.06	J/mol×K	712.50	Joback Method
cpg	605.48	J/mol×K	744.67	Joback Method
cpg	619.11	J/mol×K	776.85	Joback Method
cpg	631.96	J/mol×K	809.02	Joback Method
cpg	644.05	J/mol×K	841.19	Joback Method
cpg	655.43	J/mol×K	873.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346064&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