

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

Inchi:	InChI=1S/C16H29NO3/c1-11(2)8-7-9-20-16(19)15(13(5)6)17-14(18)10-12(3)4/h10-11,13
InchiKey:	UJOFLKIHCMJGP-UHFFFAOYSA-N
Formula:	C16H29NO3
SMILES:	CC(C)=CC(=O)NC(C(=O)OCCCC(C)C)C(C)C
Mol. weight [g/mol]:	283.41

Physical Properties

Property code	Value	Unit	Source
gf	-125.26	kJ/mol	Joback Method
hf	-585.89	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.073		Crippen Method
mcvol	250.990	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	748.53	K	Joback Method
tc	940.66	K	Joback Method
tf	380.79	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.04	J/mol×K	748.53	Joback Method
cpg	758.65	J/mol×K	780.55	Joback Method
cpg	774.33	J/mol×K	812.57	Joback Method
cpg	789.10	J/mol×K	844.59	Joback Method
cpg	802.99	J/mol×K	876.61	Joback Method
cpg	816.05	J/mol×K	908.64	Joback Method
cpg	828.30	J/mol×K	940.66	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=U346068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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