L-Valine, N-caproyl-, methyl ester

Inchi: InChI=1S/C12H23NO3/c1-5-6-7-8-10(14)13-11(9(2)3)12(15)16-4/h9,11H,5-8H2,1-4H3,(H
InchiKey: XFEUHQYGLOQDDX-UHFFFAOYSA-N
Formula: C12H23NO3
SMILES: CCCCCC(=O)NC(C(=O)OC)C(C)C
Mol. weight [g/mol]: 229.32

Physical Properties

Property code	Value	Unit	Source
hf	-738.74	kJ/mol	Cheméo Relay (1.0)
hfus	29.28	kJ/mol	Joback Method
hvap	76.79	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.53		Cheméo Relay (1.0)
logp	1.880		Crippen Method
mcvol	198.930	ml/mol	McGowan Method
rinpol	1568.00		NIST Webbook
rinpol	1568.00		NIST Webbook
tb	521.76	K	Cheméo Relay (1.0)
tc	724.59	K	Cheméo Relay (1.0)
tf	330.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.02	J/mol×K	653.41	Joback Method
cpg	560.12	J/mol×K	684.37	Joback Method
cpg	574.47	J/mol×K	715.33	Joback Method
cpg	588.06	J/mol×K	746.30	Joback Method
cpg	600.93	J/mol×K	777.26	Joback Method
cpg	613.07	J/mol×K	808.22	Joback Method
cpg	624.50	J/mol×K	839.18	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299733&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point