l-Valine, N-butyryl-, methyl ester

Inchi: InChI=1S/C10H19NO3/c1-5-6-8(12)11-9(7(2)3)10(13)14-4/h7,9H,5-6H2,1-4H3,(H,11,12)
InchiKey: LQGACXLVKKUGID-UHFFFAOYSA-N
Formula: C10H19NO3
SMILES: CCCC(=O)NC(C(=O)OC)C(C)C
Mol. weight [g/mol]: 201.26

Physical Properties

Property code	Value	Unit	Source
gf	-245.01	kJ/mol	Joback Method
hf	-564.20	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	59.42	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.100		Crippen Method
mcvol	170.750	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
tb	607.65	K	Joback Method
tc	797.00	K	Joback Method
tf	347.21	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.48	J/mol×K	607.65	Joback Method
cpg	456.44	J/mol×K	639.21	Joback Method
cpg	469.72	J/mol×K	670.77	Joback Method
cpg	482.33	J/mol×K	702.32	Joback Method
cpg	494.27	J/mol×K	733.88	Joback Method
cpg	505.56	J/mol×K	765.44	Joback Method
cpg	516.20	J/mol×K	797.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308815&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