l-Valine, N-(4-butylbenzoyl)-, methyl ester

Inchi: InChI=1S/C17H25NO3/c1-5-6-7-13-8-10-14(11-9-13)16(19)18-15(12(2)3)17(20)21-4/h8-1
InchiKey: RBRGEJUNVSRVJT-UHFFFAOYSA-N
Formula: C17H25NO3
SMILES: CCCCc1ccc(C(=O)NC(C(=O)OC)C(C)C)cc1
Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-83.29	kJ/mol	Joback Method
hf	-483.62	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	77.94	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	2.957		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
tb	799.47	K	Joback Method
tc	1007.62	K	Joback Method
tf	465.04	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.43	J/mol×K	799.47	Joback Method
cpg	749.88	J/mol×K	834.16	Joback Method
cpg	764.24	J/mol×K	868.85	Joback Method
cpg	777.56	J/mol×K	903.54	Joback Method
cpg	789.85	J/mol×K	938.23	Joback Method
cpg	801.16	J/mol×K	972.92	Joback Method
cpg	811.50	J/mol×K	1007.62	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=U299694&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