

L-Valine, N-(4-methylbenzoyl)-, butyl ester

Inchi:	InChI=1S/C17H25NO3/c1-5-6-11-21-17(20)15(12(2)3)18-16(19)14-9-7-13(4)8-10-14/h7-
InchiKey:	WHEIBZRPHEVHA-UHFFFAOYSA-N
Formula:	C17H25NO3
SMILES:	CCCCOC(=O)C(NC(=O)c1ccc(C)cc1)C(C)C
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	-4.37		Crippen Method
logp	3.093		Crippen Method
mvol	245.620	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
tb	799.47	K	Joback Method
tc	1007.62	K	Joback Method
tf	465.04	K	Joback Method
vc	0.932	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.43	J/molxK	799.47	Joback Method
cpg	749.88	J/molxK	834.16	Joback Method
cpg	764.24	J/molxK	868.85	Joback Method
cpg	777.56	J/molxK	903.54	Joback Method
cpg	789.85	J/molxK	938.23	Joback Method
cpg	801.16	J/molxK	972.92	Joback Method
cpg	811.50	J/molxK	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=U346640&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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