L-Valine, N-(2-methoxybenzoyl)-, isobutyl ester

Inchi: InChI=1S/C17H25NO4/c1-11(2)10-22-17(20)15(12(3)4)18-16(19)13-8-6-7-9-14(13)21-5/h
InchiKey: LTTONTFWPMOCJC-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: COc1ccccc1C(=O)NC(C(=O)OCC(C)C)C(C)C
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
gf	-190.73	kJ/mol	Joback Method
hf	-621.12	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	79.96	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.649		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	2258.00		NIST Webbook
rinpol	2258.00		NIST Webbook
tb	821.45	K	Joback Method
tc	1031.66	K	Joback Method
tf	472.27	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.20	J/mol×K	821.45	Joback Method
cpg	778.34	J/mol×K	856.48	Joback Method
cpg	792.31	J/mol×K	891.52	Joback Method
cpg	805.13	J/mol×K	926.55	Joback Method
cpg	816.81	J/mol×K	961.59	Joback Method
cpg	827.39	J/mol×K	996.62	Joback Method
cpg	836.87	J/mol×K	1031.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346590&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