l-Valine, N-(o-anisoyl)-, methyl ester

Inchi: InChI=1S/C14H19NO4/c1-9(2)12(14(17)19-4)15-13(16)10-7-5-6-8-11(10)18-3/h5-9,12H,
InchiKey: XOOGZBGFEMDDOY-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: COC(=O)C(NC(=O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
gf	-213.55	kJ/mol	Joback Method
hf	-553.92	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	73.67	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.623		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	753.25	K	Joback Method
tc	966.16	K	Joback Method
tf	453.46	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.94	J/mol×K	753.25	Joback Method
cpg	609.18	J/mol×K	788.73	Joback Method
cpg	622.40	J/mol×K	824.22	Joback Method
cpg	634.59	J/mol×K	859.70	Joback Method
cpg	645.78	J/mol×K	895.19	Joback Method
cpg	655.97	J/mol×K	930.67	Joback Method
cpg	665.17	J/mol×K	966.16	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U299753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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