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

Inchi: InChI=1S/C19H29NO3/c1-5-6-7-8-13-23-19(22)17(14(2)3)20-18(21)16-11-9-15(4)10-12-
InchiKey: VIRZBRHFXKCYDD-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CCCCCCOC(=O)C(NC(=O)c1ccc(C)cc1)C(C)C
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-66.45	kJ/mol	Joback Method
hf	-524.90	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.873		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook
tb	845.23	K	Joback Method
tc	1051.86	K	Joback Method
tf	487.58	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.00	J/mol×K	845.23	Joback Method
cpg	865.83	J/mol×K	879.67	Joback Method
cpg	880.54	J/mol×K	914.11	Joback Method
cpg	894.14	J/mol×K	948.54	Joback Method
cpg	906.68	J/mol×K	982.98	Joback Method
cpg	918.19	J/mol×K	1017.42	Joback Method
cpg	928.72	J/mol×K	1051.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346643&Units=SI

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