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

Inchi: InChI=1S/C16H23NO3/c1-5-10-20-16(19)14(11(2)3)17-15(18)13-8-6-12(4)7-9-13/h6-9,11
InchiKey: FDJPADAZDGHMDT-UHFFFAOYSA-N
Formula: C16H23NO3
SMILES: CCCOC(=O)C(NC(=O)c1ccc(C)cc1)C(C)C
Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-91.71	kJ/mol	Joback Method
hf	-462.98	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	75.71	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.703		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	776.59	K	Joback Method
tc	986.41	K	Joback Method
tf	453.77	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.99	J/mol×K	776.59	Joback Method
cpg	693.22	J/mol×K	811.56	Joback Method
cpg	707.38	J/mol×K	846.53	Joback Method
cpg	720.50	J/mol×K	881.50	Joback Method
cpg	732.63	J/mol×K	916.47	Joback Method
cpg	743.79	J/mol×K	951.44	Joback Method
cpg	754.00	J/mol×K	986.41	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=U346638&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