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

Inchi: InChI=1S/C19H29NO3/c1-13(2)7-6-12-23-19(22)17(14(3)4)20-18(21)16-10-8-15(5)9-11-
InchiKey: MNPSLAIKQFGFJW-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: Cc1ccc(C(=O)NC(C(=O)OCCCC(C)C)C(C)C)cc1
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-68.89	kJ/mol	Joback Method
hf	-530.18	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.729		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2351.00		NIST Webbook
rinpol	2351.00		NIST Webbook
tb	844.79	K	Joback Method
tc	1053.58	K	Joback Method
tf	472.58	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.52	J/mol×K	844.79	Joback Method
cpg	866.51	J/mol×K	879.59	Joback Method
cpg	881.32	J/mol×K	914.39	Joback Method
cpg	895.01	J/mol×K	949.19	Joback Method
cpg	907.60	J/mol×K	983.99	Joback Method
cpg	919.13	J/mol×K	1018.79	Joback Method
cpg	929.64	J/mol×K	1053.58	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=U346642&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